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TITLE OF THE INVENTION (280 characters max)

THREE-DIMENSIONAL STRUCTURE OF THE CATALYTIC DOMAIN OF ZAP-70 PROTEIN TYROSINE KINASE, METHODS, AND USE THEREOF

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THREE-DIMENSIONAL STRUCTURE OF THE CATALYTIC DOMAIN OF ZAP-70 PROTEIN TYROSINE KINASE, METHODS, AND USE THEREOF

Field of the Invention

The present invention relates to ZAP-70 protein tyrosine kinase, in particular, the three-dimensional structure of the catalytic domain of ZAP-70 protein tyrosine kinase. The invention also relates to the crystalline forms of liganded or unliganded human ZAP-70 catalytic domain. Further, the invention describes methods of making of a crystal comprising ZAP-70 and purification of the catalytic domain of ZAP-70 for use in crystallization. The invention also relates to the use of the three-dimensional structure of the catalytic domain of ZAP-70 kinase for identifying and designing ligands or low molecular weight compounds which inhibit the biological function of ZAP-70.

Background of the Invention

The protein tyrosine kinase ZAP-70 (zeta chain-associated protein of 70 kDa) plays a pivotal role in T cell activation. T cells are involved in transplant rejection, autoimmune diseases and the initiation of inflammatory responses. Activation of T cells requires engagement of the antigen-specific T cell receptor (TCR), resulting in early membrane proximal events which lead to the activation of a number of signal transduction pathways.

One of the early events of T cell activation is the phosphorylation of the TCR zeta chain and the specific association and activation of the Syk family protein tyrosine kinase ZAP-70 with the TCR via its two SH2 domains. Zeta chain-binding together with trans-phosphorylation by the src family kinase Lck leads to the activation of ZAP-70. ZAP-70 phosphorylates its specific substrate LAT (linker for activation of T cells), an adaptor molecule, which then recruits a number of downstream effector molecules. This eventually leads to the activation of early T cell genes, production of cytokines and cellular proliferation. There is ample evidence that interference with ZAP-70/LAT-mediated signaling leads to functional T cell inactivation.

Defects in ZAP-70 are the cause of selective T cell defect (STD), an autosomal recessive form of severe combined immunodeficiency characterized by a selective absence of CD-8-type T cells.

The crystal structure of the tandem SH2 domains of human ZAP-70 in complex with a peptide derived from the TCR zeta chain has been previously described by Hatada et al. (1995). This three-dimensional crystal structure of the SH2 domain has also been the subject of U.S. Patent No. 6,251,620. The disclosure of this SH2 domain has lead to efforts directed at blocking the ZAP-70 SH2 domain/zeta chain interaction. However, to date no orally active inhibitor of ZAP-70 has been described.

The present invention focuses on the three dimensional structure of the catalytic domain of ZAP-70 for inhibition of ZAP-70 since catalytic activity at the ATP-binding site can be directly inhibited. Before the disclosure of the present invention, there was no three-dimensional crystal structure of the catalytic domain of ZAP-70. With the three-dimensional structure of the catalytic domain of the human ZAP-70, identifying and designing inhibitors of ZAP-70 based on the three-dimensional structure of the catalytic domain is now possible.

Summary of the Invention

It is an object of the present invention to provide the three-dimensional structure of ZAP-70 kinase catalytic domain thereby enabling identification and design of ligands or low molecular weight molecules that specifically inhibit ZAP-70 kinase.

The present invention relates to:

(i) A crystal of the ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase with or without a ligand or low molecular weight compound;

(ii) A method of making a crystal of ZAP-70 kinase comprising the ZAP-70 kinase catalytic domain; and

(iii) Methods of using said ZAP-70 kinase crystal comprising the catalytic domain and its structural coordinates.

The three-dimensional structural information revealed from the crystal of the catalytic domain of ZAP-70 kinase can be used for structure-based drug discovery for screening, identifying and designing inhibitors of ZAP-70 kinase.

Detailed Description of the Invention

The full-length sequence of human ZAP-70 kinase is known and set forth in Genbank Accession number L05148 and SwissProt Accession number P43403, which are incorporated herein by reference.

The present invention provides ZAP-70 kinase catalytic domain in crystallized form. In particular, it provides a crystal comprising the catalytic domain of ZAP-70 kinase and a ligand bound to ZAP-70 as a complex.

In one embodiment of the present invention, a crystal of the catalytic domain of ZAP-70 kinase comprising a unit cell dimension of: a = 35.77 ± 5 Ångstroms (Å); b = 57.56 ± 5 Å; c = 80.20 ± 5 Å; α = 68.97 ± 5°; β = 89.83 ± 5°; and γ = 89.95 ± 5° is provided. Depending on the particular conditions for crystallization, the parameters characterising the unit cell may vary with a limited range, for example, a, b and c each vary by up to 5 Å and α, β and γ each vary by up to 5°. The space group of the present invention is P1 primitive triclinic.

The term "unit cell" according to the invention refers to the basic shape block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" according to the invention refers to the arrangement of symmetry elements of a crystal.

In another embodiment of the invention, a crystal of ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase in complex with a ligand is provided wherein said crystal has a three-dimensional structure characterized by the atomic structure coordinates of Table 1.

In a further embodiment of the invention, said catalytic domain of ZAP-70 kinase comprises the sequence of SEQ ID No. 2, fragment or homologue thereof.

In yet another embodiment of the invention, said catalytic domain of ZAP-70 kinase comprises at least the ATP-binding site.

Further provided by this invention is a crystal comprising the catalytic domain of ZAP-70 bound to at least one ligand or low molecular weight compound.

The term "ligand" according to the invention, refers to a molecule or group of molecules that bind to one or more specific sites of ZAP-70, preferably to the catalytic domain of ZAP-70 and most preferably to the ATP binding-site of said catalytic domain. Ligands according to the invention are preferably low molecular weight molecules.

The term "low molecular weight compound" according to the invention refers to preferably organic compounds generally having a molecular weight less than about 1000, more preferably less than about 500. Most preferably, said low molecular weight compounds or ligands inhibit ZAP-70 biological activity.

In context of a ZAP-70 inhibitor, the terms "peptide" or "peptide derivative" are intended to embrace a "peptidomimetic" or "peptide analogue" which complement the three-dimensional structure of the binding site of ZAP-70 kinase or can be designed with improved physical or chemical properties to bind with the three-dimensional binding site of the ZAP-70 kinase catalytic domain as provided in the present invention.

The term "mutant" refers to differences in the wild-type sequence of ZAP-70 kinase set forth in Genbank Accession number L05148 or SwissProt Accession number P43403 by deletion, insertion or preferably replacement of one or more selected amino acids.

According to the present invention, the term "mutant" also refers to a polypeptide, whose amino acid sequence differs from the wild-type sequence given in SEQ ID No. 2 by deletion, insertion or preferably replacement of one or more selected amino acids. For example, a ZAP-70 mutant of the catalytic domain of the present invention is preferably at least 50% homologous to SEQ ID No. 2, more preferably at least 80% homologous to SEQ ID No. 2 most preferably at least 90% homologous to SEQ ID No. 2.

A "fragment" of ZAP-70 catalytic domain according to the invention comprises more than 50% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2, more preferably at least 80% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2, most preferably at least 90% of the full-length sequence of the ZAP-70 catalytic domain according to SEQ ID No. 2.

In one embodiment of the invention, a ZAP-70 mutant of the catalytic domain may be crystallizable with or without at least one ligand.

In another embodiment of the invention, a ZAP-70 fragment of the catalytic domain may be crystallizable with or without at least one ligand.

In yet another embodiment of the invention, a method is provided wherein the catalytic domain of ZAP-70, a fragment or homologue thereof is bound to at least one ligand at any step prior to crystallization.

According to the present invention, ZAP-70 crystals are stable for at least one month, if kept under suitable conditions. Hepes pH 7.2 is identified as being suitable for the concentration of ZAP-70 without precipitation. Initially during purification, high concentrations of glycerol (30-50% $^{v}/_{v}$) are preferred, below which rapid precipitation occurs at protein concentrations in excess of 5-10 mg/mL. During the final concentration steps 1% $^{v}/_{v}$ ethylene glycol can substitute for glycerol allowing concentrations in excess of 30 mg/mL to be reached. An additional cation-exchange step is also recommended to remove incorrectly folded or unstable ZAP-70 which interferes with the concentration and crystallization process.

The purified protein ZAP-70 catalytic domain of SEQ ID No. 2, homologue or fragment thereof is advantageously obtainable according to method of the present invention by initial expression of the full-length ZAP-70 SEQ ID No. 1 flanked by protease recognition sequences. This facilitates efficient proteolytic release of the desired domain. This method is preferable to standard methods known in the art whereby the desired domain typically is isolated from the full-length protein and then expressed.

Purification of an N-terminally tagged full-length ZAP-70 using a nickel-chelating affinity column yields protein of limited purity which cannot be easily purified by additional "standard" chromatographic procedures such as ion-exchange or size-exclusion chromatography. According to the present invention, affinity chromatography using y-aminophenyl-ATP sepharose is the preferred means of purification leading to a high purity of the ZAP-70 protein. Identification of the desired ZAP-70 catalytic domain is preferably by immunochemical method, for example, Western-blotting.

In one embodiment of the invention, a method for making a crystal of a ZAP-70 kinase is provided comprising the following steps:

(i) Purification of the full-length ZAP-70 kinase (SEQ ID No. 1);

(ii) Proteolytic domain definition;

(iii) Expression of the full-length ZAP-70 kinase of SEQ ID No. 1 flanked by protease recognition sequences to facilitate proteolytic release of the desired domain of ZAP-70;

(iv) Expression of the full-length ZAP-kinase from step (iii) in a suitable host cell;

(v) Controlled proteolysis of the desired domain at protease recognition sites; and

(vi) Rapid purification of the desired ZAP-70 domain.

In a preferred embodiment of the invention, said method for making a crystal comprises the desired domain of ZAP-70 kinase domain comprising the catalytic domain of ZAP-70 kinase of SEQ ID No. 2, a fragment or homologue thereof.

According to the invention, ZAP-70 may be prepared by isolation from natural sources, e.g., cultured human cells or preferably by recombinant heterologous expression. Expression of recombinant ZAP-70 is achievable in eukaryotic or prokaryotic systems. For example, recombinant human ZAP-70 may be expressed in insect cells, such as Sf9 cells, using a suitable recombinant baculovirus system or in bacteria.

The kinase may be expressed as a fusion protein, e.g., a glutathione-S-transferase (GST) or histidine-tagged fusion protein. If desired, the fusion partner is removed before crystallization. The heterologously produced ZAP-70 to be used for crystallization is biologically active. Such ability may be determined by morphological, biochemical or viability analysis well-known in the art.

Methods for the preparation of ZAP-70 mutants are commonly known in the art. For example, ZAP-70 mutants may be prepared by expression of ZAP-70 DNA previously modified in its coding region by oligo-nucleotide directed mutagenesis.

In the present invention, purified ZAP-70 is preferably at least 90% homogeneous. Protein homogeneity is determinable according to analytical methods well-known in the art, e.g., sequence analysis, electrophoresis, spectroscopic or chromatographic techniques.

The purified protein is enzymatically active. Appropriate assays for determining ZAP-70 kinase activity towards a suitable substrate, e.g., a natural substrate or a synthetic substrate are known in the art.

In one embodiment of the invention, prior to crystallization ZAP-70 may be reacted with a low molecular weight compound or ligand which is capable of suitably binding to the ZAP-70 catalytic domain site. Preferred is a compound inhibiting ZAP-70 activity. Kinase inhibition is determinable employing assays known in the art. Suitable inhibitors include ATP-competitive kinase inhibitors which act on the catalytic domain to inhibit ZAP-70 activity.

Various methods of cystallization can be used in the claimed invention including vapor diffusion, dialysis or batch crystallization. In vapor diffusion crystallization, a small volume (i.e., a few microliters) of protein solution is mixed with a solution containing a precipitant. This mixed volume is suspended over a well containing a small amount, i.e., about 1 mL, of precipitant. Vapor diffusion from the drop to the well will result in crystal formation in the drop.

The dialysis method of crystallization utilizes a semipermeable size-exclusion membrane that retains the protein but allows small molecules (i.e., buffers and precipitants) to diffuse in and out. In dialysis, rather than concentrating the protein and the precipitant by evaporation, the precipitant is allowed to slowly diffuse through the membrane and reduce the solubility of the protein while keeping the protein concentration fixed.

The batch method generally involves the slow addition of a precipitant to an aqueous solution of protein until the solution just becomes turbid, at this point the container can be sealed and left undisturbed for a period of time until crystallization occurs. In the batch technique the precipitant and the target molecule solution are simply mixed. Supersaturation is achieved directly rather than by diffusion. Often the batch technique is performed under oil. The oil prevents evaporation and extremely small drops can be used. For this, the term "microbatch" is used. A modification of this technique is not to use paraffin oil (which prevents evaporation completely) but rather use silicone oil or a mixture of silicone and paraffin oils so that a slow evaporation is possible.

The claimed invention can encompass any and all methods of crystallization. One skilled in the art can choose any of such methods and vary the parameters such that the chosen method results in the desired crystals.

One preferred method of crystallization of ZAP-70 involves mixing a ZAP-70 solution with a "reservoir buffer", with a lower concentration of the precipitating agent necessary for crystal formation. For crystal formation, the concentration of the precipitating agent has to be increased, e.g., by addition of precipitating agent, for example, by titration, or by allowing the concentration of precipitating agent to balance by diffusion between the crystallization buffer and a reservoir buffer. Under suitable conditions such diffusion of precipitating agent occurs along the gradient of precipitating agent, e.g., from the reservoir buffer having a higher concentration of precipitating agent into the crystallization buffer having a lower concentration of precipitating agent. Diffusion may be achieved, e.g., by vapor diffusion techniques allowing diffusion of water in the common gas phase. Known techniques are, e.g., vapor diffusion methods, such as the "hanging drop" or the "sitting drop" method. In the vapor diffusion method a drop of crystallization buffer containing the protein is hanging above or sitting beside a much larger pool of reservoir buffer. Alternatively, the balancing of the precipitating agent can be achieved through a semipermeable membrane that separates the crystallization buffer from the reservoir buffer and prevents dilution of the protein into the reservoir buffer.

Formation of ZAP-70 kinase catalytic domain crystals can be achieved under various conditions which are essentially determined by the following parameters: pH, presence of salts and additives, precipitating agent, protein concentration and temperature. The pH may range, for example, from about 4.0-9.0.

The present invention also relates to a computer readable medium having stored a model of the ZAP-70 catalytic domain crystal structure. In a preferred embodiment, said model is built from all or part of the X-ray diffraction data shown in the atomic coordinates of Table 1.

The present invention provides the structure coordinates of human ZAP-70 catalytic domain. The term "structure coordinates" or "atomic coordinates" refers to mathematical coordinates derived from the mathematical equations related to the pattern obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a crystal comprising a ZAP-70 catalytic domain. The diffraction data are used to calculate an

electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Structural coordinates of a crystalline composition of this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g., a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they define. For example, data defining the three dimensional structure of a protein of the ZAP family, or portions or structurally similar homologues of such proteins, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the protein structure, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

In one embodiment of the invention, a method is provided for determining the three-dimensional structure of the catalytic domain of ZAP-70 comprising:

(i) Crystallization of ZAP-70 kinase comprising the catalytic domain of ZAP-70 (SEQ ID No. 2), fragment or homologue thereof;

(ii) Collecting X-ray diffraction data in the form of atomic coordinates for said crystal; and

(iii) Utilizing the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the catalytic domain of ZAP-70, fragment, or homologue thereof.

In another embodiment of the invention, a method is provided for determining the three-dimensional structure of a complex comprising the catalytic domain of ZAP-70 kinase (SEQ ID No. 2), fragment or homologue thereof bound to at least one ligand comprising:

(i) Obtaining X-ray diffraction data for a crystal of the complex; and

(ii) Utilizing the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the complex.

According to the present invention, a three-dimensional ZAP-70 model is obtainable from a ZAP-70 crystal comprising the catalytic domain of ZAP-70, fragment or homologue thereof. Such a model can be built or refined from all or part of the ZAP-70 kinase structure

data of the present invention using the X-ray diffraction coordinates, particularly the atomic structure coordinates of Table 1.

The knowledge obtained from the three-dimensional model of the catalytic binding site of ZAP-70 can be used in various ways. For example, it can be used to identify chemical entities, for example, small organic and bio-organic molecules, such as peptidomimetics and synthetic organic molecules that bind to ZAP-70 and preferably block or prevent a ZAP-70 mediated or associated process or event, or that act as ZAP-70 agonists. Using the three-dimensional structure of the ZAP-70 catalytic domain, the skilled artisan constructs a model of the ZAP-70. For example, every atom can be depicted as a sphere of the appropriate van der Waals radius, and a detailed surface map of the ZAP-70 catalytic domain can be constructed.

Chemical entities that have a surface that mimics the accessible surface of the catalytic binding site of ZAP-70 can be constructed by those skilled in the art. By way of example, the skilled artisan can screen three-dimensional structural databases of compounds to identify those compounds that position appropriate functional groups in similar three dimensional structural arrangement, then build combinatorial chemistry libraries around such chemical entities to identify those with high affinity to the catalytic binding site of ZAP-70.

In one embodiment of the invention, a method is provided for identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase comprising the steps of:

(i) Using the three-dimensional structure of the catalytic domain derived in whole or in part from the set of atomic coordinates in Table 1 to select a potential ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70; and

(ii) Selecting those ligands or low molecular weight compounds that bind to the catalytic domain of ZAP-70.

In another embodiment of the invention, a method is provided for identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase wherein the catalytic domain of ZAP-70 comprises at least the ATP binding site of said domain.

In yet another embodiment of the invention, a method is provided for identifying ligands which inhibit the biological activity of ZAP-70 kinase.

Ligands or small molecular compounds can be identified from screening compound databases or libraries and using a computational means to form a fitting operation to a binding site on the catalytic domain of ZAP-70 kinase. The three dimensional structure of the catalytic domain of ZAP-70 as provided in the present invention in whole or in part by the structural coordinates of Table 1, can be used together with various docking programs.

The potential inhibitory or binding effect of a chemical entity on ZAP-70 may be analyzed prior to its actual synthesis and testing by the use of computer-modeling techniques. If the theoretical structure of the given chemical entity suggests insufficient interaction and association between it and ZAP-70, the need for synthesis and testing of the chemical entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to ZAP-70. Thus, expensive and time-consuming synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of ZAP-70 may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites of ZAP-70. Thus, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with ZAP-70. This process may begin by visual inspection of, for example, the binding site on a computer screen based on the structural coordinates of Table 1 in whole or in part. Selected fragments or chemical entities may then be positioned in a variety of orientations, or "docked", within the catalytic binding site of ZAP-70. Docking may be accomplished using software such as Quanta and SyLyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER. Specialized computer programs may be of use for selecting interesting fragments or chemical entities. These programs include, for example, GRID, available from Oxford University, Oxford, UK; 5 MCSS or CATALYST, available from Molecular Simulations, Burlington, MA; AUTODOCK, available from Scripps Research Institute, La Jolla, CA; DOCK, available from University of California, San Francisco, CA; and XSITE, available from University College of London, UK.

Using molecular replacement to exploit a set of coordinates such as those of Table 1 of the invention, the structure of a crystalline ZAP-70 kinase catalytic domain or portion thereof can, for example, be bound to one or more ligands or low molecular weight compounds to form a complex.

The term "molecular replacement" refers to a method that involves generating a preliminary structural model of a crystal whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known, e.g., the ZAP-70 kinase catalytic domain coordinates within the unit cell of the unknown crystal, so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model, and combined with the observed amplitudes to give an approximated Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final accurate structure of the unknown crystal. Using the structural coordinates provided by this invention, molecular replacement may be used to determine the structural coordinates of a crystalline co complex, unknown ligand, mutant, or homolog, or of a different crystalline form of ZAP-70 kinase. Additionally, the claimed crystal and its coordinates may be used to determine the structural coordinates of a chemical entity that associates with ZAP-70.

"Homology modeling" according to the invention involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or one subdomains, such as the catalytic domain of ZAP-70 kinase. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements. Homology modeling can include rebuilding part or all of a three-dimensional structure with replace of amino acids or other components by those of the related structure to be solved.

Molecular replacement according to the present invention, uses a molecule having a known structure. The three-dimensional structure of the catalytic domain of ZAP-70 provided in whole or in part in Table 1 in a machine-readable form on a data-carrier can be used as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions in the unit cell diffract similarly. Molecular replacement involves positioning the known structure in the unit cell in the same location and orientation as the unknown structure. Once positioned, the atoms of the known structure in the unit cell are

used to calculate the structure factors that would result from a hypothetical diffraction experiment. This involves rotating the known structure in the six dimensions (three angular and three spatial dimensions) until alignment of the known structure with the experimental data is achieved. This approximate structure can be fine-tuned to yield a more accurate and often higher resolution structure using various refinement techniques. For instance, the resultant model for the structure defined by the experimental data may be subjected to rigid body refinement in which the model is subjected to limited additional rotation in the six dimensions yielding positioning shifts of under about 5%. The refined model may then be further refined using other known refinement methods. The present invention also enables homologues and mutants of ZAP-70 catalytic domain and the solving of their crystal structure. Based on the three-dimensional structure of ZAP-70 catalytic domain as provided in the present invention and using the atomic coordinates of Table 1 in whole or in part, the effects of site-specific mutations can be predicted. More specifically, the structural information provided herein permits the identification of desirable sites for amino acid modification, particularly amino acid mutation resulting in substitutional, insertional or deletional variants. Such variants may be designed to have special properties, particularly properties distinct from wild-type ZAP-70 catalytic domain, such as altered catalytic activity. Substitutions, deletions and insertions may be combined to arrive at a desired variant. Such variants can be prepared by methods well-known in the art, e.g., starting from wild-type ZAP-70 catalytic domain, or by *de novo* synthesis.

ZAP-70 catalytic domain may also crystallize in a form different from the one disclosed herein. The structural information provided, for example, in SEQ ID No. 2 and Table 1 in whole or in part, is also useful for solving the structure of other crystal forms. Furthermore, it may serve to solve the structure of a ZAP-70 catalytic domain mutant, a ZAP-70 catalytic domain co-complex or a sufficiently homologous protein.

The ZAP-70 catalytic domain structural information provided herein is useful for the design of ligands or small molecule compounds which are capable of selectively interacting with ZAP-70 catalytic domain and thereby specifically modulating the biological activity of ZAP-70. Furthermore, this information can be used to design and prepare ZAP-70 mutants, e.g., mutants with altered catalytic activity, model the three-dimensional structure and solve the crystal structure of proteins, such as ZAP-70 catalytic domain homologues, ZAP-70 catalytic domain mutants or ZAP-70 catalytic domain co-complexes, involving e.g., molecular replacement.

The present invention provides a method for designing a ligand or low molecular weight compound capable of binding with ZAP-70 catalytic domain, said method comprising:

(i) Using the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the ZAP-70 catalytic domain;

(ii) Probing said three-dimensional structural of the ZAP-70 catalytic domain with candidate ligands or low molecular weight compounds to determine which bind to the catalytic domain of ZAP-70;

(iii) Selecting those ligands or low molecular weight compounds which bind to the catalytic domain of ZAP-70; and

(iv) Optionally, modifying those ligands or low molecular weight compounds which bind to maximize physical binding properties such as solubility, affinity, specificity or potency.

Preferred is a method for designing a ZAP-70 inhibitor which interacts at the catalytic binding site. The present invention also relates to the chemical entity or ligand identified by such method. One approach enabled by this invention is the use of the structural coordinates of ZAP-70 catalytic domain to design chemical entities that bind to or associate with ZAP-70 kinase and alter the physical properties of the chemical entities in different ways. Thus, properties, such as, for example, solubility, affinity, specificity, potency, on/off rates or other binding characteristics may all be altered and/or maximized. One may design desired chemical entities by probing an ZAP-70 crystal comprising the catalytic domain with a library of different entities to determine optimal sites for interaction between candidate chemical entities and ZAP-70. For example, high-resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule adheres. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for the desired activity. Once the desired activity is obtained, the molecules can be further altered to maximize desirable properties.

The invention also contemplates computational screening of small-molecule databases or designing of chemical entities that can bind in whole or in part to ZAP-70 catalytic domain. They may also be used to solve the crystal structure of mutants, co-complexes, or the crystalline form of any other molecule homologous to, or capable of associating with, at least a portion of ZAP-70 kinase. One method that may be employed for this purpose is molecular replacement. An unknown crystal structure, which may be any

unknown structure, such as, for example, another crystal form of ZAP-70 kinase catalytic domain, an ZAP-70 kinase catalytic domain mutant or peptide, or a co-complex with ZAP-70 kinase, or any other unknown crystal of a chemical entity that associates with ZAP-70 that is of interest, may be determined using the whole of part of the structural coordinates set forth in Table 1. This method provides an accurate structural form for the unknown crystal far more quickly and efficiently than attempting to determine such information without the invention herein.

In one preferred embodiment of the invention, candidate ligands are screened in silico.

The information obtained can thus be used to obtain maximally effective inhibitors or agonists of ZAP-70. The design of chemical entities that inhibit or agonize ZAP-70 generally involves consideration of at least two factors. First, the chemical entity must be capable of physically or structurally associating with ZAP-70, preferably at the catalytic site of ZAP-70. The association may be any physical, structural, or chemical association, such as, for example, covalent or non-covalent bonding, or van der Waals, hydrophobic, or electrostatic interactions. Second, the chemical entity must be able to assume a conformation that allows it to associate with ZAP-70, preferentially at the catalytic site of ZAP-70. Although not all portions of the chemical entity will necessarily participate in the association with ZAP-70, those non-participating portions may still influence the overall conformation of the molecule. This in turn may have a significant impact on the desirability of the chemical entity. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding site.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to ZAP-70 may be tested and modified for the maximum desired characteristic(s) using computational or experimental evaluation. Various parameters can be maximized depending on the desired result. These include, but are not limited to, specificity, affinity, on/off rates, hydrophobicity, solubility and other characteristics readily identifiable by the skilled artisan.

The present invention also relates to identification of compounds which modulate ZAP-70. Preferred are compounds which inhibit ZAP-70 activity and are potentially useful for the treatment of diseases and conditions such as those which involve T cell and lymphocyte activation.

The present invention enables the use of molecular design techniques, particularly the rational drug design approach, to prepare new or improved chemical entities and compounds, including ZAP-70 inhibitors, capable of irreversibly or reversibly, modulating ZAP-70 activity. Improved entities or compounds means that these entities or compounds are superior to the "original" or parent compound they are derived from with regard to a property relevant to therapeutic use including suitability for *in vivo* administration, e.g., cellular uptake, solubility, stability against (enzymatic) degradation, binding affinity or specificity and the like. For example, on the basis on the information provided herein it is possible to specially design ZAP-70 inhibitors which covalently, or preferably non-covalently, bind to ZAP-70. Such inhibitors may act in a competitive or uncompetitive manner, bind at or close to the active site of ZAP-70 or act allosterically.

In the design of ZAP-70 modulators the following aspects should be considered:

(i) If the candidate compound is capable of physically and structurally associating with ZAP-70 kinase catalytic domain; and/or

(ii) If the compound is capable of assuming a conformation allowing it to associate with ZAP-kinase catalytic domain.

Advantageously, computer modeling techniques are used in the process of assessing these abilities for the modulator as a whole, or a fragment thereof, in order to minimize efforts in the synthesis or testing of unsuccessful candidate compounds. Specialized computer software is well-known in the art.

Another design approach is to probe a ZAP-70 catalytic domain crystal with a variety of different chemical entities to determine optimal sites for interaction between candidate ZAP-70 inhibitors and the target enzyme. Yet another possibility which arises from the present invention is to screen computationally small molecule data bases for chemical entities or compounds that are capable of binding, in whole or in part, to ZAP-70 catalytic domain. The quality of fit to the binding site may be judged e.g. by shape complementarity or by estimated interaction energy. Knowledge of the three-dimensional arrangement of the

modifications can be then utilized for the design of new ZAP-70 ligands or low molecular weight compounds, such as selective inhibitors.

Chemical entities that are capable of associating with the ZAP family member may inhibit its interaction with naturally occurring ligands of the protein and may inhibit biological functions mediated by such interaction. In the case of ZAP-70, such biological functions include activation of T cells during an immune response. Such chemical entities are potential drug candidates.

Compounds of the structures selected or designed by any of the foregoing means may be tested for their ability to bind to a ZAP family protein, inhibit the binding of a ZAP family protein to a natural or non-natural ligand therefor, and/or inhibit a biological function mediated by a ZAP family member.

The following examples serve to illustrate the present invention but should not be construed as a limitation thereof. The invention particularly relates to the specific embodiments described in these examples. Compounds first identified by any of the methods described herein are also encompassed by this invention.

EXAMPLES

Example 1: Initial Purification of Full-Length ZAP-70 Kinase

The full-length amino acid sequence of the ZAP-70 kinase is given in SEQ ID No. 1. N-terminally His_6-tagged full-length ZAP-70 kinase is expressed in Sf9 cells. This differs from the wild-type sequence in that the N-terminal is modified by insertion of a hexa-histidine sequence in between the N-terminal methionine and proline (position 2), such that this proline is now in position 8. Cell pellets are harvested and frozen at -80°C until required. A 39 g wet cell pellet is suspended in 350 mL ice-cold buffer A (50 mM sodium phosphate pH 8, containing 12 EDTA-free Complete™ protease inhibitor tablets, 10 mM β-mercaptoethanol, 10% $^{v}/_{v}$ glycerol, 0.1 mM $MnCl_2$, 10 mM imidazole and 300 mM NaCl). The cells are lysed for 3 minutes on ice using a Heidolph-Diax tissue-grinder followed by 10 strokes in a glass-teflon homogenizer. The resultant lysate is centrifuged for 45 minutes at 43,000 g at 4°C and subsequently filtered through successive glass-fiber, 1.2 µM and 0.43 µM filter membranes. This clarified supernatant is loaded at a flow-rate of 2 mL/min. onto an XK16/20 chromatography column (Amersham Biosciences) containing 20 mL

Ni-NTA-agarose (Qiagen) affinity resin equilibrated with buffer A. Once all the material has been loaded, the column is washed (at a flow-rate of 4 mL/min.) with buffer A until the UV-absorbance of the flow-through material has once again returned to baseline levels. At this point (using the same flow-rate), buffer B (25 mM Tris-HCl pH 8, 10% $^{v}/_{v}$ glycerol, 50 mM NaCl and 250 mM imidazole) is applied to the column and the peak of protein which elutes is collected. This material is loaded directly onto a 16 mL column of γ-aminophenyl-ATP sepharose equilibrated with buffer C (25 mM Tris pH 8.0 containing: 30% $^{v}/_{v}$ glycerol, 1 mM DTT, 1 mM $MgCl_2$ and 50 mM NaCl) at a flow-rate of 2 mL/min. The column is eluted by applying a gradient of 0-1 M NaCl in buffer C over 7 column volumes. The eluted peak is concentrated by ultrafiltration using a 30,000 M_r cut-off membrane (Amicon) to approximately 7 mL and further purified using a Superdex 75 (XK16/60) size-exclusion column equilibrated with buffer C (but without 50 mM NaCl). The fractions containing ZAP-70 monomer are collected and pooled prior to concentration to 2.5 mg/mL and subsequent limited proteolytic digestion.

Full-length ZAP-70 is eluted from the NTA-agarose column at a purity of approximately 60% as determined by reducing SDS-PAGE. Subsequent chromatography on a 16 mL column of γ-aminophenyl-ATP sepharose gives a rather broad peak of much higher purity which can be concentrated. Detailed analysis of this peak reveals that the earlier eluting fractions contain predominantly aggregated material and that a discrete peak towards the end of the profile contains most of the monomeric ZAP of high purity. Size-exclusion chromatography gives a major peak comprising ~90% of the protein, the remainder eluting slightly earlier in a position where dimeric or aggregated protein would be expected to elute. At this stage, the purity of the preparation is in excess of 90% and suitable for use in the limited proteolytic definition of minimal kinase domains. At this stage, highest purity is very important so as to minimize the number of additional sequences present following proteolytic digestion.

Example 2: Proteolytic Catalytic Domain Definition

ZAP-70 is incubated for 20 hours at room temperature at a 1:100 concentration ratio with the following proteases: thermolysin, carboxypeptidase A, thrombin, Arg C, Glu C, Factor Xa, Carboxypeptidase Y, chymotrpsin, Lys C, Asp N, elastase, trypsin and subtilisin (1:1 ratio). Following incubation samples are removed, subjected to reducing SDS-PAGE electrophoresis (Novex 4-20% gels, Invitrogen) and compared with non-digested controls. In the cases where faster migrating bands are observed, which are of sufficient size

(~30 kDa) to contain the catalytic domain, samples are re-run on SDS-PAGE and Western-blotted using an anti-His_6 antibody (Sigma, H-1029). This is in order to identify N-terminal and C-terminal ZAP-70 fragments (the His_6-tag is at the N-terminus, consequently forms showing anti-His_6 immunoreactivity are truncated at the C-terminus and are of no interest). Non-immunoreactive fragments are subjected to SDS-PAGE and transferred electrophoretically to PVDF membranes, the bands visualized, excised and their N-terminal sequences analyzed.

Following digestion with thermolysin, trypsin, Glu C, Asp N and elastase, faster migrating bands are observed which are of sufficient size (~30 kDa) to contain the catalytic domain. When Western-blotted against the $(His)_6$ N-terminal tag, non-immunoreactive fragments are produced by trypsin, elastase and thermolysin digestion, and are thereby defined as being C-terminal in origin. These fragments are sequenced. Trypsin and Thermolysin digestion both give a fragment with isoleucine 299 as N-terminus. Elastase produces an arginine298 fragment and thermolysin an additional leucine277 fragment. Based upon these results, ZAP-70 catalytic domains beginning with leucine277 and arginine298 are identified as being potentially suitable for crystallization.

Example 3: Cloning of PreScission™ I and II Constructs

Previous attempts to purify a number of catalytic domain constructs proved difficult due to low levels of expression of soluble protein and instability of these proteins. This instability might be, in part, due to incorrect *in vivo* folding of the isolated domains and in part due to non-optimal construct length. Therefore, the full-length ZAP-70 is expressed, flanked by the PreScission™ protease recognition sequences to facilitate efficient proteolytic release of the desired domain. Based on the results obtained from the limited proteolysis of the full-length version of ZAP-70, two constructs were made: PreScission™ I, a C-terminally His_6-tagged ZAP-70 with a PreScission™ site inserted immediately prior to leucine277 (residue 285 in construct) and PreScission II™, which contained two such sites, one upstream of arginine298 (residue 306 in construct) and one upstream of the C-terminal His_6 tag, so that this could be removed simultaneously. With the oligonucleotide MG474 and RS366 (see SEQ ID Nos. 3 and 4, respectively) and the plasmid NPL2173 encoding the wild type full-length ZAP-70 gene (Genbank Accession No. L05148), a DNA fragment is amplified which upon integration into the original NPL2173 allows the introduction of the PreScission™ cleavage site between alanine297 and arginine298. Another cleavage site is added after alanine619, preceeding the His_6-tag. The integration of the PCR fragment is

done as described earlier (see Geiser et al., *Biotechnology* (2001)). The resulting plasmid is sequenced and the correct clone called pXI347 (PlasNova NPL003792). Similarly, the plasmid pXI345 (NPL003793) is constructed by integrating the PCR fragment obtained from the NPL2173 plasmid template with the oligonucleotides MG475 and MG479 (SEQ ID Nos. 5 and 6). In pXI345, the PreScission™ cleavage site is integrated between threonine282 and leucine277 and the PreScission™ cleavage site in front of the His_6-tag is removed. The two plasmids are then introduced by transfection together with a linearized baculovirus DNA into insect cells. The numbering of amino acids is based on the sequences differs from that of Genbank Accession No. L05148, by virtue of the inclusion of the purification tag and the inserted protease recognition sequences.

The plasmids encoding the new mutants of ZAP-70 are called pXI345 and pXI347, respectively. These plasmids encode the protein ZAP PreScission™ I and ZAP PreScission™ II, respectively. As a result of the mutations, complete and highly specific proteolysis of the full-length proteins can be carried out with a high quantitative recovery of the catalytic domain of ZAP-70.

Example 4: Expression and Medium-Scale Fermentation of PreScission™ II ZAP in Baculovirus

Sf21 cells propagated in Excell 401 medium with 10% fetal calf serum are transfected with 500 ng of each recombinant transfer vector and 5 µL of linear AcNPV virus DNA (BacPAK 6) by lipofection using Bacfectin as transfection reagent (both BD/Clontech, Palo Alto, CA). After five days of incubation, the transfection supernatants are harvested and subjected to plaque assay, to derive a homogenous viral population. The isolated virus plaque picks are further amplified by infection of Sf21 cells grown in suspension in Excell 401 plus 1% FCS in roller culture, until full working virus stocks of both viruses are developed. These are again titered by plaque assays.

Large scale productions are carried out using the Wave bioreactor (Wave Biotech AG, Tagelswangen, Switzerland) at 10 *l* working volume. Sf9 cells growing in SF900 II medium (Gibco/Life Technologies) are inoculated in the Wave bag and allowed to grow for three consecutive days, reaching maximal cell densities of approximately 5×10^6 cells/mL. During the cultivation and infection process the airflow, the rocking rate and the rocking angle of the Wave reactor thermoplate are monitored and adjusted. The Sf9 cells are infected at cell densities of $1.6\text{-}4.9 \times 10^6$ cells/mL and different multiplicities of infection

(m.o.i.) between 0.5, 1 and 2 m.o.i. Simultaneously with virus addition, yeastolate (Gibco/Life Technologies) is fed to the cultures at a final concentration of 4 g/L. Cell density as well as cell viability is carefully recorded during the infection period.

Plaque assays of the amplified working virus stocks give rise to titers of 5.6 x 10^7 pfu/mL for the ZAP-70 PreScission™ I construct and 1.7 x 10^8 pfu/mL for the ZAP-70 PreScission™ II construct. Both are subsequently used for 10 L large-scale production of the two PreScission™ ZAP constructs. Both proteins are well-expressed and at least partially soluble; however, although LC-MS of NTA superflow purified PreScission™ II showed several peaks with masses of 72,404, 72,478, 72,557 and 72,635 which were thought to correspond to non-, mono-, di- and tri-phosphorylated full-length kinase, the PreScission™ I material gave such a heterogeneous LC-MS spectrum that it was impossible to assign masses, therefore all expression efforts were concentrated towards production of the PreScission™ II construct.

Example 5: Method for Optimizing Harvesting of the Sf9 Cultures

The baculovirus expression system is a lytic system; as the infection proceeds, cells die and lyse, losing their contents into the medium. In the case of the expression of proteins, such as ZAP, which are expressed intracellularly, there is a small "window" of expression in which maximal protein expression occurs before this is lost through cell lysis. Typically Western blotting will be used in conjunction with a time course of infection as well as variation of the m.o.i. to determine this time point. However, in the case of ZAP-70 PreScission™ II, the observation is made that increasing levels of expression are also accompanied by increasing levels of insoluble protein. Therefore, rapid small-scale purifications lysing 1g quantities of cells give an "on-line" readout of "purifiable" ZAP.

1 g cell pellets are removed at different time points during fermentation and lysed as described previously (but using 15 mL lysis buffer, containing 1 Complete™ EDTA-free protease inhibitor tablet). Due to the scale-down, a 0.5 mL Ni-NTA-agarose column is used and the whole process from lysis through to analytical RP-HPLC estimate of the content of isolated protein is reduced to 3-4 hours. With an optimized harvest time of 48 hours, the yield of soluble ZAP can be increased 4-fold to approximately 0.75 mg purifiable ZAP/g cells or ~7.5 mg/L culture.

Example 6: Staurosporin Binding to the ZAP-70 Kinase Catalytic Domain

ZAP-70 kinase catalytic domain (R_{298}-A_{619}; SEQ ID No. 2) defined by limited proteolysis is re-cloned as the full-length ZAP-70 kinase with a C-terminal His_6-affinity tag, but flanked by two PreScission™ protease sites. Expression is carried out using Sf9 cells grown in 10 L Wave™ bioreactors (0.45 m.o.i; 48 hours). Cells are lysed in ice-cold buffer A (50 mM $NaPO_4$, 10% $^{V}/_{V}$ glycerol, 10 mM β-mercaptoethanol, 300 mM NaCl, 10 mM Imidazole; pH 8.0) containing Complete™ EDTA-free protease inhibitor. The clarified lysate is passed over a 20 mL Ni-NTA-agarose column, the column washed with buffer A and then eluted with buffer B (25 mM Tris, 10% $^{V}/_{V}$ glycerol, 50 mM NaCl, 250 mM Imidazole; pH 8.0). All chromatography steps are either carried out on-ice or using jacketed, cooled columns. The protein is immediately de-salted into 25 mM Tris pH 8.0, containing 1 mM EDTA, 1 mM DTT, 30% $^{V}/_{V}$ glycerol and 150 mM NaCl, (using a 50 mL sephadex G-25 de-salting column; HiPrep™ 26/10 Amersham Biosciences) concentrated and staurosporin added to 2-Molar excess (by addition of the correct volume of staurosporin dissolved in DMSO to 2 mg/mL).

The protein solution (60 mL) is frozen at -80°C until required then concentrated using a 30,000 M_r cut-off ultrafiltration membrane (Amicon) down to 10-15 mL prior to size-exclusion chromatography using an XK26/90 column packed with Superdex 75™ and equilibrated with 25 mM Tris pH 8, 1 mM EDTA, 1 mM DTT, 150 mM NaCl and 30% $^{V}/_{V}$ glycerol. Fractions are collected, those corresponding to the monomeric material (ca. 40 mL) are pooled and incubated with PreScission™ protease to excise the catalytic domain from the rest of the molecule. Typically 40 mL of solution, containing 42 mg ZAP-70 PreScission™ II is digested for 135 minutes at room temperature with 420 µL PreScission™ protease solution. The cleavage reaction is monitored by reversed phase HPLC so that the reaction can be stopped as quickly as possible by immediately desalting into buffer C (20 mM $NaPO_4$, 5 mM DTT, 10 mM NaCl, 1 mM $MgCl_2$: pH 7.2). Typically 3 x 14 mL portions are applied at a flow-rate of 5 mL/min. to a HiLoad™ 26/10 column. The de-salted protein, containing a mixture of monophosphorylated (25%) and non-phosphorylated (75%) ZAP is applied to an HR10/8 cation-exchange column (Mono S™ Amersham Biosciences) equilibrated in buffer C. The column is loaded at a flow-rate of 1 mL/min. and eluted at 2 mL/min. using a 0-250 mM NaCl gradient over 512 mL.

Two major peaks are eluted, the monophosphorylated protein eluting at approximately 80 mM NaCl, the non-phosphorylated protein, slightly later at approximately 100 mM NaCl. The non- and mono-phosphorylated ZAP kinase catalytic domain peaks are collected separately, de-salted (HiLoad 26/10 column) into 20 mM HEPES pH 7.2 (containing 5 mM DTT, 1 mM $MgCl_2$, 150 mM NaCl and 1% $^{V}/_{V}$ ethyleneglycol). Staurosporine is again added to 10 Molar excess to both forms which are subsequently concentrated to 10-40 mg/mL for crystallization. This de-salting step is critical, because it removes the glycerol required for chromatography (without which, the protein precipitates) and replaces it with a low concentration of ethylene glycol which sufficiently stabilizes the protein through the concentration step, but doesn't interfere with the subsequent crystallization. 30% $^{V}/_{V}$ glycerol, on the other hand, is not suitable for crystallization as it has too large an influence on the evaporative sitting-drop process. In the case of the non-phosphorylated protein, half of the eluted peak, 36 mL is concentrated to 130 µL and a final concentration of 36 mg/mL.

By optimization of the fermentation and harvest conditions, the level of ZAP expression is increased such that the purity of ZAP PreScission™ II being eluted from the NTA column is in excess of 75% and could be adequately purified by an additional size-exclusion chromatography step prior to cleavage. Following cleavage with PreScission™ protease, two bands are observed of similar mass representing the kinase and N-terminal portions of the molecule. Cation-exchange chromatography is applied to separate the two forms. The N-terminal portion passed through the column under the conditions used. The two peaks that are eluted from the column represented two different phosphorylated forms; the monophosphorylated protein eluting at approximately 80 mM NaCl and the non-phosphorylated protein, slightly later at approximately 100 mM NaCl. These different forms are collected separately for crystallization. The yield of the mono-phosphorylated form is approximately 4-fold lower than the non-phosphorylated form, therefore most crystallography efforts concentrated on the non-phosphorylated form.

Example 7: Crystallization of PreScission™ II ZAP-70

9 mg/mL ZAP-70 non-phosphorylated catalytic kinase domain in 20 mM Hepes, 5 mM DTT, 1 mM $MgCl_2$, 150 mM NaCl, 30% glycerol and staurosporine, are used for initial crystallization screening using 96-well sitting drop crystallography plates. The first promising microcrystals are obtained with crystallization screen at 10°C. Optimization of these crystallization conditions is carried out by hanging drop vapor diffusion. The

crystallization screen at 10°C has the following crystallization conditions: 0.1 M Tris pH 7.5, 0.1 M KCl, 18% PEG 5000 monomethylether. Optimization of this crystallization condition along with optimisation of the formulation of the protein preparation results in larger crystals. Hanging drop vapor diffusion is used for optimization. Diffracting single crystals are obtained with 29 mg/mL ZAP-70 non-phosphorylated kinase domain in 20 mM Hepes, 5 mM DTT, 1 mM $MgCl_2$, 150 mM NaCl, 1% ethylene glycol and staurosporine. The optimal growth condition is: 0.1 M Tris HCl pH 7.5, 0.2 M KCl, 20% PEG 5000 monomethylether at a crystallization temperature of 10°C. Crystals appear after 1-2 days and optimal crystal size is reached after 1-2 weeks. Some single crystals grow, but most single fragments are obtained by breaking apart clusters.

Example 8: Protein Production and Crystallization of the Human ZAP-70 Protein Kinase Catalytic Domain

SEQ ID No. 2 of the human ZAP-70 protein kinase catalytic domain (non-phosphorylated) is used for crystallization. The construct comprises ZAP-70 residues 298-619 plus two additional residues from the PreScission™ cleavage site at the N-terminus and 6 residues from the PreScission™ cleavage site at the C-terminus. Small, but well-diffracting single crystals are obtained with a preparation of 29 mg/mL protein concentration and 1% ethylene glycol. Optimal growth conditions are 20% PEG 5000 monomethylether, 0.1 M Tris HCl pH 7.5, 200 mM KCl. Crystals appear after 1-2 days and optimal crystal size is reached after 1-2 weeks. Some single crystals form but most single fragments are obtained by breaking apart clusters.

Cryo-Protection

Crystals are transferred from the drop into a solution consisting of the crystallization solution (well solution) plus 20% ($^{v}/_{v}$) of glycerol and 1 mM inhibitor. Crystals mounted in a 0.05 µM cryo loop are soaked in this cryo buffer for about 10-15 seconds and then dipped into liquid propane.

Data Collection

A crystal is frozen in liquid propane and diffraction data are collected at 80 K with a MAR CCD camera at the SLS in Villingen, Switzerland. A wavelength of 0.9803 A is used. 340 images are collected with 1.0° oscillation each, using an exposure time of 6 seconds

per frame and a crystal-to-detector distance of 140 mM. Raw diffraction data are processed and scaled with the HKL program suite version 1.96.6 (see Otwinowski and Minor (1996)). Crystal data and data statistics are shown in Table 2.

Structure Determination and Refinement

The structure of the catalytic ZAP-70 kinase domain is determined by molecular replacement, using the coordinates of the LCK kinase domain x-ray structure (pdb: 3LCK, Yamaguchi and Hendrickson (1996)) as search model. Residues 245-501 of LCK are used and the phospho-Tyr residue 394 is removed for sequence similarity comparisons.

Molecular replacement is performed with the auto molecular replacement script in CCP4, using data to a maximal resolution of 4.0 Å. A 80% fraction completeness of the model with 50% fraction similarity to the input structure and 2 molecules in the asymmetric unit is expected. A clear solution is found and after an initial refinement in CNX using the standard script refine.inp the structure has an R-factor of 41.7% (R-free 43.5%). Inspection of the σ_A-weighted Fo-Fc electron density map with the program O version 7.0 (see Jones et al. (1991)) reveals a strong density for most of the C-alpha trace and most of the side chains. There are several insertions and deletions and a number of loops which are found outside the electron density and have to be corrected manually.

The model of the human ZAP-70 protein kinase catalytic domain is built and adjusted to fit the density where necessary. Insertions, mutations and deletions are made accordingly. The numbering was changed using the numbering of the SwissProt Accession No. P43403 entry for ZAP-70. The structure is refined by a number of cycles of torsion angle dynamics and energy minimization, interspersed by model re-building steps. For refinement, the "refine.inp" script of CNX 2000 is used, with the following (non-default) option: Bulk solvent correction (based on the mask method).

Cross-validation is used throughout refinement using a test set comprising 5% of the reflections. Water molecules are identified with the CNX script water_pick.inp, and selected based on difference peak height (greater than 3.0σ), hydrogen-bonding and distance criteria. NCS restrain is used for the two molecules in the asymmetric unit.

The quality of the final refined model is assessed with the programs CNX 2000 (see Brünger (1998); and Figure 7)). Pictures are made in O (see Jones et al. (1991)) or WebLab ViewerLite 3.5 (Molecular Simulations, Inc.).

Results

Small single crystals of the human ZAP-70 kinase domain are obtained with PEGMME at pH 7.5. The crystals grow in space group P1 with 2 monomers per asymmetric unit. The structure is determined by molecular replacement. The final model includes two kinase domains (residues 331-603), one molecule of staurosporine per kinase domain and 261 water molecules. It has a good geometry with a rms deviation of 0.011 Å on bond lengths and 1.3° on bond angles. The final R-factor was 0.182 (Rfree= 0.209) for all reflections between 19.26 Å and 1.90 Å.

Overall Structure

The crystal structure is extremely well defined, the full C-alpha trace between residues 331 and 603 is defined. All loops and important residues have good electron density. The B-factor distribution is as expected. The staurosporine-binding site and all interactions with the kinase domain can be described in detail. The quality of the model is good, the final R-factor is 18.2% (Rfree = 20.9%).

The ZAP-70 kinase domain folds into the typical kinase domain fold. Most of the residues are well-defined by the electron density with a few exceptions: The N-terminal residues 296-330 and the C-terminal residues 604-625 are completely disordered and therefore not visible in the X-ray structure. There are a few side chains at the surface of the molecules that do not show a well-defined electron density. A number of side chains clearly show alternating side chain positions. Those were not refined; there is only one side chain with alternating conformation close to the staurosporin-binding site, which could be of importance: SER 478.

There is an electron density of the linker region between β5 and αD. This region has an unusual sequence (Ala417 - Gly418 - Gly419 - Gly420 - Pro421) and forms part of the staurosporine binding site. This region is well ordered and the electron density is well-defined. The two important contacts (Glu 415O - N1, Ala 417N - O5).

Staurosporine-Binding Site

The binding site for staurosporine in mostly shaped by the hydrophobic side chains of the following residues: Leu344, Phe349, Val352, Val399, Met414, Met416, Ala417, Leu468. Deep in the binding pocket, two polar interactions contribute to the staurosporine binding: the main chain carbonyl oxygen of residue Glu415 binds to nitrogen N1 of staurosporine and the main chain peptide nitrogen of residue Ala417 interacts with the carbonyl oxygen O5 of staurosporine. At the other end of the staurosporine molecule there are a few polar interactions between the sugar moiety and the protein. The staurosporine methoxy group forms only van der Waals contacts, but the -N-Met group interacts with the protein through a hydrogen bridge network that is formed by a number of solvent molecules and the side chains of residue Lys424, His423, Arg465 (also involving the carboxyl oxygen of the peptide bond), Asp479 and Asn466.

An alignment (ClustalW) with some of the well-known kinase structures show that the sequence variability is rather high. Nevertheless, if the c-alpha traces get superimposed, usually a relatively good fit is noticed (53-59%).

From the alignment, many kinases have insertions or deletions compared to ZAP-70 which makes it extremely difficult to model the structure in every detail. Nevertheless, the ATP-binding site has a relatively conserved structure and is easier to model than most of the rest of the kinase domain.

Phosphorylation Sites

Phosphorylation of residues in the activation segment causes conformational changes in the catalytic kinase domain that lead to the correct positioning of substrate binding residues and catalytic residues, and relief of steric blocking to enable access of substrate to the catalytic site.

The kinase domain crystallized here, is not phosphorylated. However, ZAP-70 contains a number of tyrosine residues, which can be phosphorylated *in vivo* and contribute to the regulation of the kinase activity and adaptor molecule binding. Due to the fact, that we are targeting the ATP binding site, it should not be a huge drawback that we only have the structure of the non-activated/phosphorylated kinase domain.

The phosphorylation sites 474, 492, 493, 597, and 598 are defined in the X-ray structure. Tyrosine 492 and 493 are both located in the activation loop. Transphosphorylation of Tyrosine 493 by Lck leads to activation of ZAP-70 (see Chan et al. (1995); Wange et al. (1995); Mège et al. (1996)). This tyrosine residue corresponds to tyrosine1163 of the insulin receptor kinase domain which causes upon transphosphorylation, a major conformational change of the activation loop (see Hubbard (1997)). It is thus likely that the structure of the corresponding activation loop of ZAP-70 phosphorylated at tyrosine493 will be different than the one shown here. The role of tyrosine492 is less clear. A negative regulatory function has been proposed (see Chan et al. (1995)). Tyrosine474 is required for association with the Shc adapter, which couples T cell receptor signaling to the Ras pathway (see Pacini et al. (1998)). The surface exposed tyrosine474 is located at the beginning of the β8 segment, close to the following activation segment. Tyrosine597 and tyrosine598 located at the surface of the protein near to the C-terminus are supposed to be involved in regulating the functional activity of ZAP-70 possibly by inhibitory proteins (see Zeitlmann et al. (1998)).

Claims

1. A crystal of the ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase with a unit cell dimension of: a = 35.77 ± 5 Ångstroms (Å); b = 57.56 ± 5 Å; c = 80.20 ± 5 Å; α = 68.97 ± 5°; β = 89.83 ± 5°; and γ = 89.95 ± 5°.

2. A crystal of the ZAP-70 kinase comprising the catalytic domain of ZAP-70 kinase wherein said catalytic domain has a three-dimensional structure comprising the atomic structure coordinates of Table 1.

3. A crystal of Claims 1 or 2, wherein the catalytic domain of ZAP-70 kinase comprises the sequence of SEQ ID No. 2, fragment or a homologue thereof.

4. A crystal of Claim 3, wherein the catalytic domain of ZAP-70 kinase comprises at least the ATP-binding site.

5. A crystal of any of Claims 1-4 bound to at least one ligand or low molecular weight compound.

6. A computer readable medium comprising data storage material encoded with computer readable data wherein said data comprises the atomic coordinates of Table 1 comprising the catalytic domain of ZAP-70 kinase.

7. A method for making a crystal of a ZAP-70 kinase comprising the steps of:

(i) Purification of the full-length ZAP-70 kinase of SEQ ID No. 1;

(ii) Proteolytic domain definition;

(iii) Expression of the full-length ZAP-70 kinase of SEQ ID No. 1 flanked by protease recognition sequences to facilitate proteolytic release of the desired domain of ZAP-70;

(iv) Expression of the full-length ZAP-70 kinase of step (iii) in a suitable host cell;

(v) Controlled proteolysis of the desired domain at protease recognition sites; and

(vi) Rapid purification of the desired ZAP-70 domain.

8. A method according to Claim 7, wherein the domain comprises the catalytic domain of ZAP-70 kinase of SEQ ID No. 2, fragment or a homologue thereof.

9. A method according to Claims 7 and 8, wherein the catalytic domain of ZAP-70, fragment or homologue thereof is bound to at least one ligand or low molecule weight chemical compound at any step prior to crystallization.

10. A method of determining the three-dimensional structure of the catalytic domain of ZAP-70 comprising:

(i) Crystallization of ZAP-70 kinase comprising the catalytic domain of ZAP-70 (SEQ ID No. 2), fragment or homologue thereof; and

(ii) Utilizing the atomic coordinates of Table 1 in whole or in part to determine the three-dimensional structure of the catalytic domain of ZAP-70, fragment or homologue thereof.

11. A method for determining the three-dimensional structure of a complex comprising the catalytic domain of ZAP-70 kinase (SEQ ID No. 2), fragment or homologue thereof bound to at least one ligand comprising:

(i) Obtaining X-ray diffraction data for crystals of the complex; and

(ii) Utilizing the atomic coordinates of Table 1 in whole or in part to define the three-dimensional structure of the complex.

12. A method of identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase comprising the steps of:

(i) Using the three dimensional structure of the catalytic domain of ZAP-70 kinase derived in whole or in part from the set of atomic coordinates in Table 1 to select a potential ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70; and

(ii) Selecting those ligands or low molecular weight compounds that bind to the catalytic domain of ZAP-70.

13. A method of identifying a ligand or low molecular weight compound that binds to the catalytic domain of ZAP-70 kinase according to Claim 11, wherein the catalytic domain of ZAP-70 kinase comprises at least the ATP-binding site of said domain.

14. A method of Claims 12 and 13 for use in selecting ligands which inhibit the biological activity of ZAP-70 kinase.

15. A method of designing a ligand or low molecular weight compound capable of binding to ZAP-70 catalytic domain comprising:

(i) Using the atomic coodinates of Table 1 in whole or in part to determine the three dimensional structure of ZAP-70 catalytic domain;

(ii) Probing the catalytic domain of ZAP-70 with candidate ligands or low molecular weight compounds to determine which bind to the catalytic domain of ZAP-70;

(iii) Selecting those ligands or low molecular weight compounds which bind to the catalytic domain of ZAP-70; and

(iv) Modifying those ligands or low molecular weight compounds which bind to maximize physical binding properties such as solubility, affinity, specificity or potency.

16. A method according to Claim 15, wherein the candidate ligands or low molecular weight compounds are screened *in silico*.

17. A method according to Claims 15-16 for use in designing ligands which inhibit the biological activity of ZAP-70 kinase.

18. A pharmaceutical composition comprising a ligand identified by the methods of Claims 12-14 for use of treatment of diseases and conditions involving T-cell and lymphocyte activation.

Table 1. Atomic Coordinates of ZAP-70 Catalytic Domain with Staurosporine

```
REMARK   3   PROGRAM     : CNX 2000.1
REMARK   3   AUTHORS     : Brunger, Adams, Clore, Delano,
REMARK   3                 Gros, Grosse-Kunstleve, Jiang,
REMARK   3                 Kuszewski, Nilges, Pannu, Read,
REMARK   3                 Rice, Simonson, Warren
REMARK   3                   and
REMARK   3                 Molecular Simulations Inc.,
REMARK   3                 (Badger, Berard, Kumar, Szalma,
REMARK   3                  Yip).
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.90
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  19.26
REMARK   3   DATA CUTOFF                (SIGMA(F)) : 0.0
REMARK   3   DATA CUTOFF HIGH             (ABS(F)) :   933984.58
REMARK   3   DATA CUTOFF LOW              (ABS(F)) :     0.000000
REMARK   3   COMPLETENESS (WORKING+TEST)    (%) : 96.7
REMARK   3   NUMBER OF REFLECTIONS                : 45463
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD              : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION      : RANDOM
REMARK   3   R VALUE                (WORKING SET) : 0.182
REMARK   3   FREE R VALUE                         : 0.209
REMARK   3   FREE R VALUE TEST SET SIZE     (%)   :  5.0
REMARK   3   FREE R VALUE TEST SET COUNT          :  2284
REMARK   3   ESTIMATED ERROR OF FREE R VALUE      : 0.004
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED                 :   6
REMARK   3   BIN RESOLUTION RANGE HIGH           (A)  : 1.90
REMARK   3   BIN RESOLUTION RANGE LOW            (A)  : 2.02
REMARK   3   BIN COMPLETENESS (WORKING+TEST)     (%)  : 93.7
REMARK   3   REFLECTIONS IN BIN     (WORKING SET)     :  6918
REMARK   3   BIN R VALUE            (WORKING SET)     : 0.195
REMARK   3   BIN FREE R VALUE                         : 0.241
REMARK   3   BIN FREE R VALUE TEST SET SIZE     (%)   :  5.2
REMARK   3   BIN FREE R VALUE TEST SET COUNT          :   378
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE      : 0.012
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 4739
REMARK   3   NUCLEIC ACID ATOMS       :    0
REMARK   3   HETEROGEN ATOMS          :    0
REMARK   3   SOLVENT ATOMS            :    0
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT                (A**2) : 24.1
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 35.0
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :  0.16
REMARK   3    B22 (A**2) : -1.31
REMARK   3    B33 (A**2) :  1.15
REMARK   3    B12 (A**2) :  0.00
REMARK   3    B13 (A**2) :  2.08
REMARK   3    B23 (A**2) : -1.25
REMARK   3
REMARK   3  BULK SOLVENT MODELING.
REMARK   3   METHOD USED : FLAT MODEL
REMARK   3   KSOL        : 0.38494
REMARK   3   BSOL        : 52.9849 (A**2)
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT        (A) : 0.19
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REMARK   3   ESD FROM SIGMAA                (A) : 0.01
REMARK   3   LOW RESOLUTION CUTOFF          (A) : 5.00
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT      (A) : 0.22
REMARK   3   ESD FROM C-V SIGMAA            (A) : 0.11
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                   (A) : 0.011
REMARK   3   BOND ANGLES                (DEGREES) : 1.3
REMARK   3   DIHEDRAL ANGLES            (DEGREES) : 21.4
REMARK   3   IMPROPER ANGLES            (DEGREES) : 0.91
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) :  3.56 ;  1.50
REMARK   3   MAIN-CHAIN ANGLE             (A**2) :  4.55 ;  2.00
REMARK   3   SIDE-CHAIN BOND              (A**2) :  4.82 ;  2.00
REMARK   3   SIDE-CHAIN ANGLE             (A**2) :  6.37 ;  2.50
REMARK   3
REMARK   3  NCS MODEL : NONE
REMARK   3
REMARK   3  NCS RESTRAINTS.                          RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL              (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR            (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1   : MSI_CNX_TOPPAR/protein_rep.param
REMARK   3  PARAMETER FILE  2   : MSI_CNX_TOPPAR/water_rep.param
REMARK   3  PARAMETER FILE  3   : stu.param
REMARK   3  TOPOLOGY FILE  1    : MSI_CNX_TOPPAR/protein.top
REMARK   3  TOPOLOGY FILE  2    : MSI_CNX_TOPPAR/water.top
REMARK   3  TOPOLOGY FILE  3    : stu.toppar
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
SEQRES   1 A  273  PHE LEU LYS ARG ASP ASN LEU LEU ILE ALA ASP ILE GLU
SEQRES   2 A  273  LEU GLY CYS GLY ASN PHE GLY SER VAL ARG GLN GLY VAL
SEQRES   3 A  273  TYR ARG MET ARG LYS LYS GLN ILE ASP VAL ALA ILE LYS
SEQRES   4 A  273  VAL LEU LYS GLN GLY THR GLU LYS ALA ASP THR GLU GLU
SEQRES   5 A  273  MET MET ARG GLU ALA GLN ILE MET HIS GLN LEU ASP ASN
SEQRES   6 A  273  PRO TYR ILE VAL ARG LEU ILE GLY VAL CYS GLN ALA GLU
SEQRES   7 A  273  ALA LEU MET LEU VAL MET GLU MET ALA GLY GLY GLY PRO
SEQRES   8 A  273  LEU HIS LYS PHE LEU VAL GLY LYS ARG GLU GLU ILE PRO
SEQRES   9 A  273  VAL SER ASN VAL ALA GLU LEU LEU HIS GLN VAL SER MET
SEQRES  10 A  273  GLY MET LYS TYR LEU GLU GLU LYS ASN PHE VAL HIS ARG
SEQRES  11 A  273  ASP LEU ALA ALA ARG ASN VAL LEU LEU VAL ASN ARG HIS
SEQRES  12 A  273  TYR ALA LYS ILE SER ASP PHE GLY LEU SER LYS ALA LEU
SEQRES  13 A  273  GLY ALA ASP ASP SER TYR TYR THR ALA ARG SER ALA GLY
SEQRES  14 A  273  LYS TRP PRO LEU LYS TRP TYR ALA PRO GLU CYS ILE ASN
SEQRES  15 A  273  PHE ARG LYS PHE SER SER ARG SER ASP VAL TRP SER TYR
SEQRES  16 A  273  GLY VAL THR MET TRP GLU ALA LEU SER TYR GLY GLN LYS
SEQRES  17 A  273  PRO TYR LYS LYS MET LYS GLY PRO GLU VAL MET ALA PHE
SEQRES  18 A  273  ILE GLU GLN GLY LYS ARG MET GLU CYS PRO PRO GLU CYS
SEQRES  19 A  273  PRO PRO GLU LEU TYR ALA LEU MET SER ASP CYS TRP ILE
SEQRES  20 A  273  TYR LYS TRP GLU ASP ARG PRO ASP PHE LEU THR VAL GLU
SEQRES  21 A  273  GLN ARG MET ARG ALA CYS TYR TYR SER LEU ALA SER LYS
SEQRES   1 B  273  PHE LEU LYS ARG ASP ASN LEU LEU ILE ALA ASP ILE GLU
SEQRES   2 B  273  LEU GLY CYS GLY ASN PHE GLY SER VAL ARG GLN GLY VAL
SEQRES   3 B  273  TYR ARG MET ARG LYS LYS GLN ILE ASP VAL ALA ILE LYS
SEQRES   4 B  273  VAL LEU LYS GLN GLY THR GLU LYS ALA ASP THR GLU GLU
SEQRES   5 B  273  MET MET ARG GLU ALA GLN ILE MET HIS GLN LEU ASP ASN
SEQRES   6 B  273  PRO TYR ILE VAL ARG LEU ILE GLY VAL CYS GLN ALA GLU
SEQRES   7 B  273  ALA LEU MET LEU VAL MET GLU MET ALA GLY GLY GLY PRO
SEQRES   8 B  273  LEU HIS LYS PHE LEU VAL GLY LYS ARG GLU GLU ILE PRO
SEQRES   9 B  273  VAL SER ASN VAL ALA GLU LEU LEU HIS GLN VAL SER MET
SEQRES  10 B  273  GLY MET LYS TYR LEU GLU GLU LYS ASN PHE VAL HIS ARG
SEQRES  11 B  273  ASP LEU ALA ALA ARG ASN VAL LEU LEU VAL ASN ARG HIS
SEQRES  12 B  273  TYR ALA LYS ILE SER ASP PHE GLY LEU SER LYS ALA LEU
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SEQRES  13 B  273  GLY ALA ASP ASP SER TYR TYR THR ALA ARG SER ALA GLY
SEQRES  14 B  273  LYS TRP PRO LEU LYS TRP TYR ALA PRO GLU CYS ILE ASN
SEQRES  15 B  273  PHE ARG LYS PHE SER SER ARG SER ASP VAL TRP SER TYR
SEQRES  16 B  273  GLY VAL THR MET TRP GLU ALA LEU SER TYR GLY GLN LYS
SEQRES  17 B  273  PRO TYR LYS LYS MET LYS GLY PRO GLU VAL MET ALA PHE
SEQRES  18 B  273  ILE GLU GLN GLY LYS ARG MET GLU CYS PRO PRO GLU CYS
SEQRES  19 B  273  PRO PRO GLU LEU TYR ALA LEU MET SER ASP CYS TRP ILE
SEQRES  20 B  273  TYR LYS TRP GLU ASP ARG PRO ASP PHE LEU THR VAL GLU
SEQRES  21 B  273  GLN ARG MET ARG ALA CYS TYR TYR SER LEU ALA SER LYS
SEQRES   1 C    1  STU
SEQRES   1 D    1  STU
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SEQRES  19 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  20 S  261  TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP TIP
SEQRES  21 S  261  TIP
CRYST1   35.768   57.562   80.211  68.97  89.83  89.95 P 1           5
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.027958 -0.000024 -0.000079        0.00000
SCALE2      0.000000  0.017373 -0.006679        0.00000
SCALE3      0.000000  0.000000  0.013357        0.00000
ATOM      1  CB  PHE A 331      -0.844 -23.839 -13.860  1.00 47.80           C
ATOM      2  CG  PHE A 331      -0.845 -24.256 -12.414  1.00 49.69           C
ATOM      3  CD1 PHE A 331      -2.033 -24.319 -11.699  1.00 53.17           C
ATOM      4  CD2 PHE A 331       0.342 -24.562 -11.764  1.00 47.25           C
ATOM      5  CE1 PHE A 331      -2.041 -24.679 -10.359  1.00 48.16           C
ATOM      6  CE2 PHE A 331       0.344 -24.924 -10.421  1.00 51.80           C
ATOM      7  CZ  PHE A 331      -0.849 -24.982  -9.720  1.00 49.42           C
ATOM      8  C   PHE A 331      -0.689 -21.905 -15.439  1.00 47.08           C
ATOM      9  O   PHE A 331      -1.461 -21.795 -16.393  1.00 48.72           O
ATOM     10  N   PHE A 331      -2.670 -22.155 -13.939  1.00 46.43           N
ATOM     11  CA  PHE A 331      -1.196 -22.366 -14.074  1.00 43.11           C
ATOM     12  N   LEU A 332       0.610 -21.631 -15.514  1.00 40.15           N
ATOM     13  CA  LEU A 332       1.245 -21.166 -16.746  1.00 42.89           C
ATOM     14  CB  LEU A 332       1.949 -19.824 -16.490  1.00 42.08           C
ATOM     15  CG  LEU A 332       1.135 -18.662 -15.894  1.00 41.32           C
ATOM     16  CD1 LEU A 332       2.088 -17.561 -15.415  1.00 36.46           C
ATOM     17  CD2 LEU A 332       0.146 -18.116 -16.931  1.00 40.99           C
ATOM     18  C   LEU A 332       2.273 -22.195 -17.207  1.00 41.99           C
ATOM     19  O   LEU A 332       2.746 -23.003 -16.416  1.00 41.81           O
ATOM     20  N   LYS A 333       2.615 -22.171 -18.492  1.00 42.98           N
ATOM     21  CA  LYS A 333       3.614 -23.091 -19.018  1.00 44.97           C
ATOM     22  CB  LYS A 333       3.495 -23.221 -20.537  1.00 45.64           C
ATOM     23  CG  LYS A 333       2.201 -23.857 -20.971  1.00 51.28           C
ATOM     24  CD  LYS A 333       2.310 -24.340 -22.408  1.00 57.41           C
ATOM     25  CE  LYS A 333       1.041 -25.067 -22.838  1.00 58.44           C
ATOM     26  NZ  LYS A 333       1.189 -25.656 -24.206  1.00 62.81           N
ATOM     27  C   LYS A 333       4.998 -22.577 -18.673  1.00 43.59           C
ATOM     28  O   LYS A 333       5.321 -21.420 -18.952  1.00 39.19           O
ATOM     29  N   ARG A 334       5.813 -23.455 -18.097  1.00 37.84           N
```

ATOM	30	CA	ARG	A	334	7.167	-23.109	-17.698	1.00	42.87	C
ATOM	31	CB	ARG	A	334	7.831	-24.309	-17.015	1.00	46.05	C
ATOM	32	CG	ARG	A	334	9.264	-24.063	-16.553	1.00	41.63	C
ATOM	33	CD	ARG	A	334	9.303	-23.119	-15.368	1.00	37.46	C
ATOM	34	NE	ARG	A	334	10.669	-22.817	-14.947	1.00	37.67	N
ATOM	35	CZ	ARG	A	334	11.471	-21.972	-15.580	1.00	41.87	C
ATOM	36	NH1	ARG	A	334	11.038	-21.340	-16.671	1.00	38.44	N
ATOM	37	NH2	ARG	A	334	12.699	-21.747	-15.121	1.00	41.45	N
ATOM	38	C	ARG	A	334	7.999	-22.691	-18.905	1.00	42.10	C
ATOM	39	O	ARG	A	334	8.981	-21.961	-18.769	1.00	39.41	O
ATOM	40	N	ASP	A	335	7.587	-23.169	-20.077	1.00	43.76	N
ATOM	41	CA	ASP	A	335	8.274	-22.895	-21.340	1.00	44.45	C
ATOM	42	CB	ASP	A	335	7.718	-23.822	-22.423	1.00	52.46	C
ATOM	43	CG	ASP	A	335	7.632	-25.261	-21.962	1.00	55.02	C
ATOM	44	OD1	ASP	A	335	8.688	-25.925	-21.897	1.00	60.98	O
ATOM	45	OD2	ASP	A	335	6.512	-25.723	-21.643	1.00	62.85	O
ATOM	46	C	ASP	A	335	8.110	-21.455	-21.789	1.00	43.50	C
ATOM	47	O	ASP	A	335	8.904	-20.951	-22.594	1.00	41.39	O
ATOM	48	N	ASN	A	336	7.079	-20.783	-21.287	1.00	30.71	N
ATOM	49	CA	ASN	A	336	6.837	-19.407	-21.673	1.00	33.27	C
ATOM	50	CB	ASN	A	336	5.341	-19.129	-21.723	1.00	36.84	C
ATOM	51	CG	ASN	A	336	4.647	-19.915	-22.809	1.00	49.26	C
ATOM	52	OD1	ASN	A	336	5.193	-20.109	-23.899	1.00	49.53	O
ATOM	53	ND2	ASN	A	336	3.426	-20.351	-22.527	1.00	48.43	N
ATOM	54	C	ASN	A	336	7.494	-18.421	-20.731	1.00	28.53	C
ATOM	55	O	ASN	A	336	7.363	-17.210	-20.895	1.00	30.15	O
ATOM	56	N	LEU	A	337	8.203	-18.948	-19.749	1.00	32.36	N
ATOM	57	CA	LEU	A	337	8.855	-18.115	-18.750	1.00	34.27	C
ATOM	58	CB	LEU	A	337	8.365	-18.518	-17.350	1.00	30.14	C
ATOM	59	CG	LEU	A	337	8.920	-17.781	-16.125	1.00	28.85	C
ATOM	60	CD1	LEU	A	337	8.290	-16.416	-16.039	1.00	27.73	C
ATOM	61	CD2	LEU	A	337	8.586	-18.559	-14.850	1.00	35.78	C
ATOM	62	C	LEU	A	337	10.380	-18.202	-18.800	1.00	31.60	C
ATOM	63	O	LEU	A	337	10.956	-19.279	-18.875	1.00	32.32	O
ATOM	64	N	LEU	A	338	11.032	-17.051	-18.741	1.00	25.65	N
ATOM	65	CA	LEU	A	338	12.486	-17.006	-18.731	1.00	24.94	C
ATOM	66	CB	LEU	A	338	13.020	-16.257	-19.977	1.00	28.20	C
ATOM	67	CG	LEU	A	338	14.554	-16.272	-20.089	1.00	30.23	C
ATOM	68	CD1	LEU	A	338	15.028	-17.702	-20.306	1.00	33.75	C
ATOM	69	CD2	LEU	A	338	15.012	-15.400	-21.245	1.00	31.10	C
ATOM	70	C	LEU	A	338	12.855	-16.235	-17.465	1.00	29.76	C
ATOM	71	O	LEU	A	338	12.624	-15.030	-17.384	1.00	30.99	O
ATOM	72	N	ILE	A	339	13.401	-16.933	-16.471	1.00	30.96	N
ATOM	73	CA	ILE	A	339	13.763	-16.266	-15.219	1.00	29.19	C
ATOM	74	CB	ILE	A	339	13.645	-17.230	-14.011	1.00	33.77	C
ATOM	75	CG2	ILE	A	339	13.912	-16.458	-12.704	1.00	30.52	C
ATOM	76	CG1	ILE	A	339	12.267	-17.901	-14.025	1.00	32.27	C
ATOM	77	CD1	ILE	A	339	12.057	-18.955	-12.960	1.00	38.69	C
ATOM	78	C	ILE	A	339	15.185	-15.743	-15.277	1.00	31.14	C
ATOM	79	O	ILE	A	339	16.119	-16.500	-15.534	1.00	34.19	O
ATOM	80	N	ALA	A	340	15.347	-14.448	-15.029	1.00	29.75	N
ATOM	81	CA	ALA	A	340	16.676	-13.843	-15.055	1.00	34.31	C
ATOM	82	CB	ALA	A	340	16.569	-12.342	-15.334	1.00	32.66	C
ATOM	83	C	ALA	A	340	17.406	-14.090	-13.736	1.00	36.59	C
ATOM	84	O	ALA	A	340	16.788	-14.463	-12.724	1.00	34.25	O
ATOM	85	N	ASP	A	341	18.718	-13.901	-13.745	1.00	33.86	N
ATOM	86	CA	ASP	A	341	19.514	-14.093	-12.542	1.00	37.73	C
ATOM	87	CB	ASP	A	341	20.924	-14.582	-12.911	1.00	45.65	C
ATOM	88	CG	ASP	A	341	21.639	-15.259	-11.738	1.00	56.30	C
ATOM	89	OD1	ASP	A	341	21.455	-14.811	-10.588	1.00	59.09	O
ATOM	90	OD2	ASP	A	341	22.399	-16.234	-11.966	1.00	62.33	O
ATOM	91	C	ASP	A	341	19.594	-12.739	-11.850	1.00	43.58	C
ATOM	92	O	ASP	A	341	20.683	-12.245	-11.562	1.00	44.94	O
ATOM	93	N	ILE	A	342	18.434	-12.134	-11.595	1.00	36.82	N
ATOM	94	CA	ILE	A	342	18.349	-10.829	-10.954	1.00	35.58	C
ATOM	95	CB	ILE	A	342	17.894	-9.763	-11.969	1.00	38.49	C
ATOM	96	CG2	ILE	A	342	17.708	-8.407	-11.281	1.00	43.25	C
ATOM	97	CG1	ILE	A	342	18.912	-9.675	-13.106	1.00	36.31	C

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ATOM     98  CD1 ILE A 342      18.468  -8.769 -14.239  1.00 46.83           C
ATOM     99  C   ILE A 342      17.327 -10.911  -9.825  1.00 37.22           C
ATOM    100  O   ILE A 342      16.214 -11.364 -10.037  1.00 31.02           O
ATOM    101  N   GLU A 343      17.710 -10.475  -8.633  1.00 33.59           N
ATOM    102  CA  GLU A 343      16.816 -10.526  -7.485  1.00 36.18           C
ATOM    103  CB  GLU A 343      17.566 -11.064  -6.264  1.00 36.52           C
ATOM    104  CG  GLU A 343      16.713 -11.123  -5.003  1.00 40.70           C
ATOM    105  CD  GLU A 343      17.356 -11.929  -3.889  1.00 48.49           C
ATOM    106  OE1 GLU A 343      17.391 -13.175  -3.992  1.00 50.24           O
ATOM    107  OE2 GLU A 343      17.833 -11.314  -2.915  1.00 51.47           O
ATOM    108  C   GLU A 343      16.263  -9.143  -7.180  1.00 37.22           C
ATOM    109  O   GLU A 343      17.031  -8.236  -6.890  1.00 32.38           O
ATOM    110  N   LEU A 344      14.937  -8.989  -7.246  1.00 25.47           N
ATOM    111  CA  LEU A 344      14.317  -7.693  -6.969  1.00 23.40           C
ATOM    112  CB  LEU A 344      12.916  -7.594  -7.644  1.00 23.43           C
ATOM    113  CG  LEU A 344      12.969  -7.779  -9.161  1.00 32.75           C
ATOM    114  CD1 LEU A 344      11.538  -7.940  -9.704  1.00 27.03           C
ATOM    115  CD2 LEU A 344      13.684  -6.585  -9.819  1.00 32.92           C
ATOM    116  C   LEU A 344      14.185  -7.494  -5.471  1.00 25.30           C
ATOM    117  O   LEU A 344      14.236  -6.365  -4.982  1.00 29.77           O
ATOM    118  N   GLY A 345      13.997  -8.591  -4.736  1.00 25.68           N
ATOM    119  CA  GLY A 345      13.884  -8.500  -3.296  1.00 27.74           C
ATOM    120  C   GLY A 345      13.777  -9.886  -2.700  1.00 29.98           C
ATOM    121  O   GLY A 345      13.835 -10.872  -3.418  1.00 31.85           O
ATOM    122  N   CYS A 346      13.638  -9.976  -1.382  1.00 29.57           N
ATOM    123  CA  CYS A 346      13.498 -11.286  -0.755  1.00 32.14           C
ATOM    124  CB  CYS A 346      14.867 -11.885  -0.465  1.00 38.98           C
ATOM    125  SG  CYS A 346      15.741 -10.909   0.749  1.00 43.33           S
ATOM    126  C   CYS A 346      12.719 -11.167   0.544  1.00 36.85           C
ATOM    127  O   CYS A 346      12.395 -10.063   0.978  1.00 38.86           O
ATOM    128  N   GLY A 347      12.428 -12.316   1.142  1.00 36.28           N
ATOM    129  CA  GLY A 347      11.704 -12.369   2.402  1.00 35.52           C
ATOM    130  C   GLY A 347      11.923 -13.746   2.997  1.00 35.81           C
ATOM    131  O   GLY A 347      12.671 -14.541   2.435  1.00 32.94           O
ATOM    132  N   ASN A 348      11.272 -14.040   4.116  1.00 39.18           N
ATOM    133  CA  ASN A 348      11.406 -15.350   4.749  1.00 42.21           C
ATOM    134  CB  ASN A 348      10.644 -15.387   6.080  1.00 48.61           C
ATOM    135  CG  ASN A 348      11.277 -14.514   7.131  1.00 53.37           C
ATOM    136  OD1 ASN A 348      12.442 -14.702   7.492  1.00 56.08           O
ATOM    137  ND2 ASN A 348      10.516 -13.546   7.635  1.00 59.19           N
ATOM    138  C   ASN A 348      10.881 -16.464   3.852  1.00 39.31           C
ATOM    139  O   ASN A 348      11.275 -17.619   3.996  1.00 39.22           O
ATOM    140  N   PHE A 349       9.980 -16.116   2.933  1.00 35.86           N
ATOM    141  CA  PHE A 349       9.404 -17.095   2.016  1.00 32.64           C
ATOM    142  CB  PHE A 349       8.143 -16.518   1.352  1.00 37.33           C
ATOM    143  CG  PHE A 349       8.416 -15.318   0.467  1.00 33.86           C
ATOM    144  CD1 PHE A 349       9.019 -15.475  -0.777  1.00 38.44           C
ATOM    145  CD2 PHE A 349       8.121 -14.031   0.905  1.00 37.11           C
ATOM    146  CE1 PHE A 349       9.332 -14.360  -1.573  1.00 37.32           C
ATOM    147  CE2 PHE A 349       8.427 -12.917   0.123  1.00 38.27           C
ATOM    148  CZ  PHE A 349       9.036 -13.082  -1.120  1.00 36.15           C
ATOM    149  C   PHE A 349      10.394 -17.491   0.919  1.00 33.34           C
ATOM    150  O   PHE A 349      10.333 -18.586   0.367  1.00 36.04           O
ATOM    151  N   GLY A 350      11.287 -16.575   0.574  1.00 36.72           N
ATOM    152  CA  GLY A 350      12.234 -16.848  -0.490  1.00 29.36           C
ATOM    153  C   GLY A 350      12.627 -15.562  -1.166  1.00 32.07           C
ATOM    154  O   GLY A 350      12.959 -14.591  -0.506  1.00 37.38           O
ATOM    155  N   SER A 351      12.595 -15.526  -2.493  1.00 34.36           N
ATOM    156  CA  SER A 351      12.993 -14.304  -3.151  1.00 33.56           C
ATOM    157  CB  SER A 351      14.439 -14.414  -3.605  1.00 39.89           C
ATOM    158  OG  SER A 351      14.564 -15.336  -4.654  1.00 38.83           O
ATOM    159  C   SER A 351      12.093 -13.929  -4.318  1.00 25.34           C
ATOM    160  O   SER A 351      11.246 -14.703  -4.741  1.00 30.57           O
ATOM    161  N   VAL A 352      12.282 -12.719  -4.812  1.00 25.32           N
ATOM    162  CA  VAL A 352      11.484 -12.243  -5.934  1.00 27.67           C
ATOM    163  CB  VAL A 352      10.777 -10.928  -5.596  1.00 26.27           C
ATOM    164  CG1 VAL A 352       9.988 -10.443  -6.807  1.00 28.62           C
ATOM    165  CG2 VAL A 352       9.846 -11.136  -4.387  1.00 25.93           C
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ATOM	166	C	VAL	A	352	12.504	-12.002	-7.022	1.00	24.75	C
ATOM	167	O	VAL	A	352	13.416	-11.177	-6.862	1.00	26.64	O
ATOM	168	N	ARG	A	353	12.334	-12.720	-8.124	1.00	21.24	N
ATOM	169	CA	ARG	A	353	13.259	-12.640	-9.253	1.00	24.10	C
ATOM	170	CB	ARG	A	353	13.643	-14.052	-9.721	1.00	24.70	C
ATOM	171	CG	ARG	A	353	14.430	-14.913	-8.722	1.00	41.94	C
ATOM	172	CD	ARG	A	353	15.851	-14.401	-8.516	1.00	48.67	C
ATOM	173	NE	ARG	A	353	16.805	-15.494	-8.339	1.00	56.82	N
ATOM	174	CZ	ARG	A	353	17.287	-16.243	-9.330	1.00	59.51	C
ATOM	175	NH1	ARG	A	353	16.913	-16.024	-10.585	1.00	54.48	N
ATOM	176	NH2	ARG	A	353	18.140	-17.226	-9.065	1.00	58.82	N
ATOM	177	C	ARG	A	353	12.625	-11.910	-10.430	1.00	30.05	C
ATOM	178	O	ARG	A	353	11.403	-11.914	-10.605	1.00	32.28	O
ATOM	179	N	GLN	A	354	13.461	-11.288	-11.245	1.00	26.89	N
ATOM	180	CA	GLN	A	354	12.954	-10.605	-12.429	1.00	21.13	C
ATOM	181	CB	GLN	A	354	13.886	-9.449	-12.813	1.00	27.45	C
ATOM	182	CG	GLN	A	354	13.394	-8.651	-14.005	1.00	33.20	C
ATOM	183	CD	GLN	A	354	14.196	-7.386	-14.228	1.00	35.81	C
ATOM	184	OE1	GLN	A	354	14.929	-6.932	-13.344	1.00	32.36	O
ATOM	185	NE2	GLN	A	354	14.048	-6.798	-15.410	1.00	38.36	N
ATOM	186	C	GLN	A	354	12.954	-11.650	-13.537	1.00	26.03	C
ATOM	187	O	GLN	A	354	13.773	-12.580	-13.516	1.00	27.62	O
ATOM	188	N	GLY	A	355	12.044	-11.498	-14.498	1.00	23.59	N
ATOM	189	CA	GLY	A	355	12.005	-12.421	-15.612	1.00	23.56	C
ATOM	190	C	GLY	A	355	11.167	-11.834	-16.740	1.00	28.28	C
ATOM	191	O	GLY	A	355	10.786	-10.665	-16.702	1.00	25.55	O
ATOM	192	N	VAL	A	356	10.901	-12.664	-17.755	1.00	28.64	N
ATOM	193	CA	VAL	A	356	10.074	-12.264	-18.883	1.00	29.66	C
ATOM	194	CB	VAL	A	356	10.921	-12.045	-20.174	1.00	34.30	C
ATOM	195	CG1	VAL	A	356	10.005	-11.659	-21.351	1.00	32.44	C
ATOM	196	CG2	VAL	A	356	11.931	-10.977	-19.919	1.00	29.39	C
ATOM	197	C	VAL	A	356	9.108	-13.402	-19.127	1.00	23.76	C
ATOM	198	O	VAL	A	356	9.485	-14.569	-19.033	1.00	26.47	O
ATOM	199	N	TYR	A	357	7.859	-13.064	-19.438	1.00	28.83	N
ATOM	200	CA	TYR	A	357	6.847	-14.082	-19.703	1.00	29.55	C
ATOM	201	CB	TYR	A	357	5.697	-14.003	-18.693	1.00	32.75	C
ATOM	202	CG	TYR	A	357	4.603	-14.999	-18.981	1.00	31.78	C
ATOM	203	CD1	TYR	A	357	4.766	-16.355	-18.702	1.00	33.06	C
ATOM	204	CE1	TYR	A	357	3.761	-17.287	-19.010	1.00	38.12	C
ATOM	205	CD2	TYR	A	357	3.417	-14.587	-19.575	1.00	38.71	C
ATOM	206	CE2	TYR	A	357	2.410	-15.504	-19.887	1.00	39.65	C
ATOM	207	CZ	TYR	A	357	2.587	-16.844	-19.601	1.00	39.40	C
ATOM	208	OH	TYR	A	357	1.577	-17.722	-19.904	1.00	48.05	O
ATOM	209	C	TYR	A	357	6.291	-13.846	-21.098	1.00	33.01	C
ATOM	210	O	TYR	A	357	6.038	-12.699	-21.484	1.00	34.42	O
ATOM	211	N	ARG	A	358	6.093	-14.925	-21.845	1.00	40.49	N
ATOM	212	CA	ARG	A	358	5.582	-14.797	-23.201	1.00	43.14	C
ATOM	213	CB	ARG	A	358	6.303	-15.787	-24.128	1.00	42.64	C
ATOM	214	CG	ARG	A	358	5.804	-15.762	-25.580	1.00	47.94	C
ATOM	215	CD	ARG	A	358	6.599	-16.738	-26.435	1.00	46.49	C
ATOM	216	NE	ARG	A	358	6.555	-18.096	-25.898	1.00	48.83	N
ATOM	217	CZ	ARG	A	358	7.470	-19.024	-26.159	1.00	47.27	C
ATOM	218	NH1	ARG	A	358	8.496	-18.736	-26.947	1.00	48.46	N
ATOM	219	NH2	ARG	A	358	7.365	-20.239	-25.636	1.00	49.08	N
ATOM	220	C	ARG	A	358	4.083	-15.023	-23.299	1.00	37.81	C
ATOM	221	O	ARG	A	358	3.602	-16.102	-22.983	1.00	39.13	O
ATOM	222	N	MET	A	359	3.361	-13.984	-23.712	1.00	48.72	N
ATOM	223	CA	MET	A	359	1.917	-14.072	-23.926	1.00	52.67	C
ATOM	224	CB	MET	A	359	1.185	-12.898	-23.284	1.00	56.85	C
ATOM	225	CG	MET	A	359	1.487	-12.704	-21.817	1.00	59.91	C
ATOM	226	SD	MET	A	359	0.442	-11.450	-21.068	1.00	68.40	S
ATOM	227	CE	MET	A	359	1.094	-9.949	-21.845	1.00	66.35	C
ATOM	228	C	MET	A	359	1.810	-13.963	-25.443	1.00	57.95	C
ATOM	229	O	MET	A	359	2.127	-12.913	-26.006	1.00	66.19	O
ATOM	230	N	ARG	A	360	1.393	-15.043	-26.097	1.00	60.89	N
ATOM	231	CA	ARG	A	360	1.282	-15.079	-27.561	1.00	63.37	C
ATOM	232	CB	ARG	A	360	0.383	-16.246	-27.994	1.00	64.54	C
ATOM	233	CG	ARG	A	360	0.960	-17.616	-27.623	1.00	65.69	C

ATOM	234	CD	ARG	A	360	2.353	-17.786	-28.231	1.00	65.62	C
ATOM	235	NE	ARG	A	360	3.255	-18.567	-27.384	1.00	65.60	N
ATOM	236	CZ	ARG	A	360	3.082	-19.851	-27.070	1.00	63.16	C
ATOM	237	NH1	ARG	A	360	2.027	-20.525	-27.527	1.00	62.71	N
ATOM	238	NH2	ARG	A	360	3.977	-20.470	-26.309	1.00	62.89	N
ATOM	239	C	ARG	A	360	0.788	-13.774	-28.175	1.00	63.27	C
ATOM	240	O	ARG	A	360	-0.417	-13.601	-28.401	1.00	68.94	O
ATOM	241	N	LYS	A	361	1.743	-12.878	-28.448	1.00	59.53	N
ATOM	242	CA	LYS	A	361	1.511	-11.549	-29.022	1.00	56.77	C
ATOM	243	CB	LYS	A	361	0.219	-10.938	-28.461	1.00	60.05	C
ATOM	244	CG	LYS	A	361	0.226	-10.722	-26.950	1.00	60.48	C
ATOM	245	CD	LYS	A	361	-1.174	-10.402	-26.409	1.00	62.81	C
ATOM	246	CE	LYS	A	361	-1.771	-9.144	-27.036	1.00	64.09	C
ATOM	247	NZ	LYS	A	361	-3.154	-8.872	-26.526	1.00	65.39	N
ATOM	248	C	LYS	A	361	2.701	-10.647	-28.659	1.00	61.19	C
ATOM	249	O	LYS	A	361	3.151	-9.813	-29.464	1.00	60.48	O
ATOM	250	N	LYS	A	362	3.204	-10.819	-27.436	1.00	52.69	N
ATOM	251	CA	LYS	A	362	4.334	-10.035	-26.949	1.00	54.92	C
ATOM	252	CB	LYS	A	362	3.901	-8.588	-26.737	1.00	56.85	C
ATOM	253	CG	LYS	A	362	2.785	-8.432	-25.728	1.00	53.56	C
ATOM	254	CD	LYS	A	362	2.334	-6.986	-25.680	1.00	58.19	C
ATOM	255	CE	LYS	A	362	1.452	-6.738	-24.479	1.00	60.02	C
ATOM	256	NZ	LYS	A	362	0.281	-7.656	-24.462	1.00	59.99	N
ATOM	257	C	LYS	A	362	4.900	-10.601	-25.642	1.00	48.81	C
ATOM	258	O	LYS	A	362	4.298	-11.460	-25.015	1.00	48.05	O
ATOM	259	N	GLN	A	363	6.069	-10.119	-25.241	1.00	51.22	N
ATOM	260	CA	GLN	A	363	6.682	-10.594	-24.007	1.00	49.77	C
ATOM	261	CB	GLN	A	363	8.095	-11.132	-24.267	1.00	54.46	C
ATOM	262	CG	GLN	A	363	8.154	-12.259	-25.286	1.00	52.95	C
ATOM	263	CD	GLN	A	363	9.545	-12.865	-25.397	1.00	54.97	C
ATOM	264	OE1	GLN	A	363	10.550	-12.189	-25.172	1.00	58.63	O
ATOM	265	NE2	GLN	A	363	9.606	-14.135	-25.764	1.00	57.23	N
ATOM	266	C	GLN	A	363	6.737	-9.459	-23.014	1.00	46.14	C
ATOM	267	O	GLN	A	363	7.198	-8.366	-23.329	1.00	52.39	O
ATOM	268	N	ILE	A	364	6.269	-9.716	-21.799	1.00	38.56	N
ATOM	269	CA	ILE	A	364	6.266	-8.671	-20.796	1.00	38.92	C
ATOM	270	CB	ILE	A	364	4.865	-8.450	-20.233	1.00	46.04	C
ATOM	271	CG2	ILE	A	364	3.907	-8.072	-21.353	1.00	42.34	C
ATOM	272	CG1	ILE	A	364	4.388	-9.715	-19.542	1.00	38.48	C
ATOM	273	CD1	ILE	A	364	3.262	-9.453	-18.591	1.00	46.96	C
ATOM	274	C	ILE	A	364	7.199	-8.974	-19.643	1.00	35.15	C
ATOM	275	O	ILE	A	364	7.473	-10.142	-19.337	1.00	29.70	O
ATOM	276	N	ASP	A	365	7.685	-7.922	-19.005	1.00	32.92	N
ATOM	277	CA	ASP	A	365	8.577	-8.086	-17.872	1.00	31.39	C
ATOM	278	CB	ASP	A	365	9.253	-6.762	-17.552	1.00	35.51	C
ATOM	279	CG	ASP	A	365	10.142	-6.278	-18.685	1.00	40.87	C
ATOM	280	OD1	ASP	A	365	10.983	-7.066	-19.158	1.00	44.73	O
ATOM	281	OD2	ASP	A	365	9.997	-5.102	-19.089	1.00	47.04	O
ATOM	282	C	ASP	A	365	7.728	-8.520	-16.663	1.00	31.78	C
ATOM	283	O	ASP	A	365	6.656	-7.977	-16.442	1.00	31.99	O
ATOM	284	N	VAL	A	366	8.214	-9.484	-15.889	1.00	25.27	N
ATOM	285	CA	VAL	A	366	7.472	-9.945	-14.722	1.00	24.77	C
ATOM	286	CB	VAL	A	366	6.831	-11.346	-14.959	1.00	21.57	C
ATOM	287	CG1	VAL	A	366	5.761	-11.282	-16.055	1.00	23.23	C
ATOM	288	CG2	VAL	A	366	7.923	-12.389	-15.281	1.00	24.77	C
ATOM	289	C	VAL	A	366	8.365	-10.061	-13.486	1.00	26.20	C
ATOM	290	O	VAL	A	366	9.576	-10.016	-13.580	1.00	26.40	O
ATOM	291	N	ALA	A	367	7.742	-10.156	-12.315	1.00	23.36	N
ATOM	292	CA	ALA	A	367	8.471	-10.354	-11.074	1.00	27.38	C
ATOM	293	CB	ALA	A	367	8.166	-9.227	-10.067	1.00	25.34	C
ATOM	294	C	ALA	A	367	7.911	-11.716	-10.615	1.00	29.93	C
ATOM	295	O	ALA	A	367	6.703	-11.961	-10.667	1.00	29.39	O
ATOM	296	N	ILE	A	368	8.799	-12.603	-10.203	1.00	26.23	N
ATOM	297	CA	ILE	A	368	8.418	-13.962	-9.814	1.00	26.26	C
ATOM	298	CB	ILE	A	368	9.182	-15.008	-10.677	1.00	29.25	C
ATOM	299	CG2	ILE	A	368	8.711	-16.425	-10.355	1.00	27.48	C
ATOM	300	CG1	ILE	A	368	8.974	-14.706	-12.168	1.00	26.91	C
ATOM	301	CD1	ILE	A	368	10.261	-14.543	-12.965	1.00	35.91	C

ATOM	302	C	ILE	A	368	8.744	-14.257	-8.352	1.00	26.03	C
ATOM	303	O	ILE	A	368	9.893	-14.229	-7.959	1.00	24.27	O
ATOM	304	N	LYS	A	369	7.720	-14.539	-7.561	1.00	25.90	N
ATOM	305	CA	LYS	A	369	7.953	-14.862	-6.156	1.00	26.26	C
ATOM	306	CB	LYS	A	369	6.691	-14.547	-5.344	1.00	25.23	C
ATOM	307	CG	LYS	A	369	6.822	-14.795	-3.870	1.00	31.86	C
ATOM	308	CD	LYS	A	369	5.509	-14.423	-3.158	1.00	34.03	C
ATOM	309	CE	LYS	A	369	5.538	-14.876	-1.716	1.00	39.65	C
ATOM	310	NZ	LYS	A	369	4.354	-14.402	-0.910	1.00	31.37	N
ATOM	311	C	LYS	A	369	8.298	-16.361	-6.140	1.00	27.61	C
ATOM	312	O	LYS	A	369	7.474	-17.219	-6.492	1.00	29.29	O
ATOM	313	N	VAL	A	370	9.532	-16.674	-5.764	1.00	26.60	N
ATOM	314	CA	VAL	A	370	9.990	-18.065	-5.766	1.00	28.07	C
ATOM	315	CB	VAL	A	370	11.355	-18.200	-6.481	1.00	33.07	C
ATOM	316	CG1	VAL	A	370	11.721	-19.667	-6.633	1.00	38.83	C
ATOM	317	CG2	VAL	A	370	11.315	-17.506	-7.841	1.00	30.80	C
ATOM	318	C	VAL	A	370	10.154	-18.575	-4.340	1.00	33.33	C
ATOM	319	O	VAL	A	370	10.920	-18.021	-3.558	1.00	31.84	O
ATOM	320	N	LEU	A	371	9.433	-19.627	-3.996	1.00	32.52	N
ATOM	321	CA	LEU	A	371	9.555	-20.176	-2.653	1.00	37.90	C
ATOM	322	CB	LEU	A	371	8.383	-21.111	-2.357	1.00	40.40	C
ATOM	323	CG	LEU	A	371	7.003	-20.462	-2.304	1.00	38.75	C
ATOM	324	CD1	LEU	A	371	5.960	-21.529	-2.018	1.00	42.86	C
ATOM	325	CD2	LEU	A	371	6.987	-19.389	-1.236	1.00	40.03	C
ATOM	326	C	LEU	A	371	10.877	-20.936	-2.523	1.00	41.99	C
ATOM	327	O	LEU	A	371	11.250	-21.709	-3.413	1.00	37.51	O
ATOM	328	N	LYS	A	372	11.571	-20.717	-1.411	1.00	40.63	N
ATOM	329	CA	LYS	A	372	12.847	-21.374	-1.151	1.00	47.85	C
ATOM	330	CB	LYS	A	372	13.430	-20.879	0.176	1.00	49.15	C
ATOM	331	CG	LYS	A	372	12.538	-21.128	1.390	1.00	52.08	C
ATOM	332	CD	LYS	A	372	13.153	-20.548	2.655	1.00	53.51	C
ATOM	333	CE	LYS	A	372	12.283	-20.840	3.875	1.00	55.66	C
ATOM	334	NZ	LYS	A	372	12.885	-20.313	5.137	1.00	59.56	N
ATOM	335	C	LYS	A	372	12.691	-22.894	-1.121	1.00	52.35	C
ATOM	336	O	LYS	A	372	11.591	-23.413	-0.941	1.00	50.37	O
ATOM	337	N	GLN	A	373	13.799	-23.605	-1.312	1.00	59.78	N
ATOM	338	CA	GLN	A	373	13.780	-25.067	-1.304	1.00	59.32	C
ATOM	339	CB	GLN	A	373	15.115	-25.606	-1.835	1.00	63.62	C
ATOM	340	CG	GLN	A	373	15.155	-27.116	-2.051	1.00	66.24	C
ATOM	341	CD	GLN	A	373	14.191	-27.586	-3.134	1.00	71.01	C
ATOM	342	OE1	GLN	A	373	12.970	-27.465	-2.995	1.00	69.21	O
ATOM	343	NE2	GLN	A	373	14.739	-28.129	-4.219	1.00	68.75	N
ATOM	344	C	GLN	A	373	13.529	-25.584	0.116	1.00	60.87	C
ATOM	345	O	GLN	A	373	14.088	-25.061	1.085	1.00	58.13	O
ATOM	346	N	GLY	A	374	12.673	-26.595	0.238	1.00	60.47	N
ATOM	347	CA	GLY	A	374	12.378	-27.150	1.548	1.00	63.49	C
ATOM	348	C	GLY	A	374	11.112	-26.589	2.169	1.00	65.45	C
ATOM	349	O	GLY	A	374	10.744	-26.960	3.287	1.00	64.91	O
ATOM	350	N	THR	A	375	10.448	-25.694	1.440	1.00	64.08	N
ATOM	351	CA	THR	A	375	9.211	-25.073	1.910	1.00	62.35	C
ATOM	352	CB	THR	A	375	8.624	-24.117	0.837	1.00	61.07	C
ATOM	353	OG1	THR	A	375	9.499	-22.997	0.658	1.00	58.51	O
ATOM	354	CG2	THR	A	375	7.251	-23.619	1.255	1.00	60.44	C
ATOM	355	C	THR	A	375	8.164	-26.128	2.254	1.00	60.26	C
ATOM	356	O	THR	A	375	7.812	-26.960	1.420	1.00	61.11	O
ATOM	357	N	GLU	A	376	7.669	-26.085	3.486	1.00	61.48	N
ATOM	358	CA	GLU	A	376	6.659	-27.038	3.937	1.00	63.66	C
ATOM	359	CB	GLU	A	376	6.395	-26.854	5.431	1.00	65.34	C
ATOM	360	CG	GLU	A	376	5.410	-27.863	6.011	1.00	70.83	C
ATOM	361	CD	GLU	A	376	5.443	-27.905	7.531	1.00	74.17	C
ATOM	362	OE1	GLU	A	376	5.151	-26.868	8.174	1.00	71.51	O
ATOM	363	OE2	GLU	A	376	5.765	-28.983	8.083	1.00	74.47	O
ATOM	364	C	GLU	A	376	5.365	-26.847	3.157	1.00	64.69	C
ATOM	365	O	GLU	A	376	5.071	-25.745	2.693	1.00	62.88	O
ATOM	366	N	LYS	A	377	4.595	-27.921	3.015	1.00	60.06	N
ATOM	367	CA	LYS	A	377	3.339	-27.860	2.282	1.00	61.26	C
ATOM	368	CB	LYS	A	377	2.637	-29.219	2.317	1.00	66.02	C
ATOM	369	CG	LYS	A	377	1.309	-29.238	1.575	1.00	65.91	C

ATOM	370	CD	LYS	A	377	0.916	-30.656	1.195	1.00	71.13	C
ATOM	371	CE	LYS	A	377	-0.343	-30.679	0.335	1.00	69.84	C
ATOM	372	NZ	LYS	A	377	-0.745	-32.070	-0.037	1.00	70.61	N
ATOM	373	C	LYS	A	377	2.405	-26.794	2.833	1.00	60.41	C
ATOM	374	O	LYS	A	377	1.535	-26.293	2.121	1.00	58.25	O
ATOM	375	N	ALA	A	378	2.586	-26.456	4.104	1.00	60.36	N
ATOM	376	CA	ALA	A	378	1.757	-25.450	4.756	1.00	60.42	C
ATOM	377	CB	ALA	A	378	2.126	-25.353	6.232	1.00	60.96	C
ATOM	378	C	ALA	A	378	1.914	-24.083	4.090	1.00	58.57	C
ATOM	379	O	ALA	A	378	0.928	-23.406	3.792	1.00	58.22	O
ATOM	380	N	ASP	A	379	3.159	-23.690	3.849	1.00	58.14	N
ATOM	381	CA	ASP	A	379	3.446	-22.398	3.237	1.00	59.61	C
ATOM	382	CB	ASP	A	379	4.889	-21.999	3.513	1.00	61.20	C
ATOM	383	CG	ASP	A	379	5.387	-22.533	4.841	1.00	69.25	C
ATOM	384	OD1	ASP	A	379	4.801	-22.184	5.892	1.00	70.24	O
ATOM	385	OD2	ASP	A	379	6.367	-23.313	4.831	1.00	70.38	O
ATOM	386	C	ASP	A	379	3.198	-22.428	1.730	1.00	57.10	C
ATOM	387	O	ASP	A	379	2.944	-21.394	1.118	1.00	54.39	O
ATOM	388	N	THR	A	380	3.279	-23.616	1.137	1.00	51.67	N
ATOM	389	CA	THR	A	380	3.023	-23.766	-0.287	1.00	52.52	C
ATOM	390	CB	THR	A	380	3.350	-25.193	-0.755	1.00	53.17	C
ATOM	391	OG1	THR	A	380	4.769	-25.392	-0.709	1.00	55.35	O
ATOM	392	CG2	THR	A	380	2.858	-25.411	-2.168	1.00	57.49	C
ATOM	393	C	THR	A	380	1.536	-23.488	-0.506	1.00	53.07	C
ATOM	394	O	THR	A	380	1.142	-22.808	-1.449	1.00	46.30	O
ATOM	395	N	GLU	A	381	0.714	-24.029	0.386	1.00	48.31	N
ATOM	396	CA	GLU	A	381	-0.726	-23.844	0.310	1.00	49.46	C
ATOM	397	CB	GLU	A	381	-1.421	-24.722	1.355	1.00	55.95	C
ATOM	398	CG	GLU	A	381	-2.487	-25.651	0.794	1.00	57.87	C
ATOM	399	CD	GLU	A	381	-1.909	-26.852	0.064	1.00	66.85	C
ATOM	400	OE1	GLU	A	381	-1.256	-26.663	-0.988	1.00	67.42	O
ATOM	401	OE2	GLU	A	381	-2.112	-27.992	0.547	1.00	68.23	O
ATOM	402	C	GLU	A	381	-1.025	-22.371	0.585	1.00	47.48	C
ATOM	403	O	GLU	A	381	-1.985	-21.810	0.061	1.00	44.28	O
ATOM	404	N	GLU	A	382	-0.181	-21.752	1.404	1.00	42.74	N
ATOM	405	CA	GLU	A	382	-0.332	-20.346	1.764	1.00	44.98	C
ATOM	406	CB	GLU	A	382	0.697	-19.989	2.828	1.00	50.35	C
ATOM	407	CG	GLU	A	382	0.552	-18.600	3.407	1.00	54.73	C
ATOM	408	CD	GLU	A	382	1.479	-18.376	4.593	1.00	61.59	C
ATOM	409	OE1	GLU	A	382	2.719	-18.344	4.400	1.00	67.89	O
ATOM	410	OE2	GLU	A	382	0.963	-18.241	5.726	1.00	66.58	O
ATOM	411	C	GLU	A	382	-0.150	-19.453	0.531	1.00	43.95	C
ATOM	412	O	GLU	A	382	-0.893	-18.490	0.331	1.00	37.04	O
ATOM	413	N	MET	A	383	0.847	-19.772	-0.288	1.00	38.03	N
ATOM	414	CA	MET	A	383	1.063	-18.984	-1.490	1.00	37.01	C
ATOM	415	CB	MET	A	383	2.425	-19.295	-2.124	1.00	37.76	C
ATOM	416	CG	MET	A	383	2.854	-18.195	-3.108	1.00	44.12	C
ATOM	417	SD	MET	A	383	4.495	-18.400	-3.806	1.00	45.79	S
ATOM	418	CE	MET	A	383	4.148	-19.720	-4.849	1.00	27.93	C
ATOM	419	C	MET	A	383	-0.054	-19.244	-2.490	1.00	33.92	C
ATOM	420	O	MET	A	383	-0.365	-18.389	-3.311	1.00	28.10	O
ATOM	421	N	MET	A	384	-0.672	-20.423	-2.432	1.00	30.29	N
ATOM	422	CA	MET	A	384	-1.770	-20.707	-3.346	1.00	35.41	C
ATOM	423	CB	MET	A	384	-2.129	-22.190	-3.338	1.00	37.28	C
ATOM	424	CG	MET	A	384	-1.098	-23.082	-4.013	1.00	44.29	C
ATOM	425	SD	MET	A	384	-0.753	-22.611	-5.733	1.00	47.70	S
ATOM	426	CE	MET	A	384	-2.394	-22.740	-6.491	1.00	43.44	C
ATOM	427	C	MET	A	384	-2.988	-19.871	-2.970	1.00	32.30	C
ATOM	428	O	MET	A	384	-3.746	-19.436	-3.838	1.00	32.40	O
ATOM	429	N	ARG	A	385	-3.186	-19.642	-1.680	1.00	36.42	N
ATOM	430	CA	ARG	A	385	-4.305	-18.814	-1.250	1.00	36.70	C
ATOM	431	CB	ARG	A	385	-4.470	-18.850	0.270	1.00	41.37	C
ATOM	432	CG	ARG	A	385	-5.158	-20.106	0.794	1.00	46.84	C
ATOM	433	CD	ARG	A	385	-5.569	-19.933	2.261	1.00	45.50	C
ATOM	434	NE	ARG	A	385	-4.432	-20.021	3.171	1.00	49.04	N
ATOM	435	CZ	ARG	A	385	-3.842	-21.165	3.508	1.00	48.50	C
ATOM	436	NH1	ARG	A	385	-4.291	-22.309	3.007	1.00	48.28	N
ATOM	437	NH2	ARG	A	385	-2.806	-21.167	4.334	1.00	48.88	N

ATOM	438	C	ARG	A	385	-4.048	-17.381	-1.712	1.00	32.36	C
ATOM	439	O	ARG	A	385	-4.970	-16.666	-2.088	1.00	34.82	O
ATOM	440	N	GLU	A	386	-2.780	-16.976	-1.692	1.00	29.93	N
ATOM	441	CA	GLU	A	386	-2.395	-15.633	-2.125	1.00	29.40	C
ATOM	442	CB	GLU	A	386	-0.893	-15.413	-1.881	1.00	28.50	C
ATOM	443	CG	GLU	A	386	-0.333	-14.053	-2.289	1.00	33.73	C
ATOM	444	CD	GLU	A	386	1.178	-13.959	-2.037	1.00	35.02	C
ATOM	445	OE1	GLU	A	386	1.750	-14.956	-1.548	1.00	36.68	O
ATOM	446	OE2	GLU	A	386	1.797	-12.905	-2.343	1.00	36.70	O
ATOM	447	C	GLU	A	386	-2.713	-15.481	-3.615	1.00	27.47	C
ATOM	448	O	GLU	A	386	-3.215	-14.437	-4.060	1.00	28.61	O
ATOM	449	N	ALA	A	387	-2.412	-16.525	-4.377	1.00	30.23	N
ATOM	450	CA	ALA	A	387	-2.673	-16.488	-5.806	1.00	33.30	C
ATOM	451	CB	ALA	A	387	-2.097	-17.735	-6.484	1.00	32.95	C
ATOM	452	C	ALA	A	387	-4.194	-16.386	-6.031	1.00	30.92	C
ATOM	453	O	ALA	A	387	-4.638	-15.601	-6.843	1.00	33.56	O
ATOM	454	N	GLN	A	388	-4.975	-17.163	-5.286	1.00	31.73	N
ATOM	455	CA	GLN	A	388	-6.440	-17.119	-5.438	1.00	36.88	C
ATOM	456	CB	GLN	A	388	-7.108	-18.109	-4.461	1.00	39.93	C
ATOM	457	CG	GLN	A	388	-6.725	-19.564	-4.694	1.00	48.53	C
ATOM	458	CD	GLN	A	388	-7.273	-20.496	-3.619	1.00	55.51	C
ATOM	459	OE1	GLN	A	388	-8.480	-20.524	-3.360	1.00	58.01	O
ATOM	460	NE2	GLN	A	388	-6.383	-21.263	-2.982	1.00	52.09	N
ATOM	461	C	GLN	A	388	-7.001	-15.711	-5.201	1.00	33.60	C
ATOM	462	O	GLN	A	388	-7.904	-15.271	-5.902	1.00	31.97	O
ATOM	463	N	ILE	A	389	-6.469	-15.004	-4.204	1.00	30.12	N
ATOM	464	CA	ILE	A	389	-6.914	-13.643	-3.905	1.00	25.06	C
ATOM	465	CB	ILE	A	389	-6.305	-13.132	-2.569	1.00	28.76	C
ATOM	466	CG2	ILE	A	389	-6.507	-11.626	-2.426	1.00	29.47	C
ATOM	467	CG1	ILE	A	389	-6.964	-13.868	-1.398	1.00	37.06	C
ATOM	468	CD1	ILE	A	389	-6.359	-13.540	-0.058	1.00	34.67	C
ATOM	469	C	ILE	A	389	-6.524	-12.696	-5.022	1.00	26.55	C
ATOM	470	O	ILE	A	389	-7.326	-11.901	-5.494	1.00	30.71	O
ATOM	471	N	MET	A	390	-5.278	-12.779	-5.461	1.00	27.33	N
ATOM	472	CA	MET	A	390	-4.845	-11.910	-6.529	1.00	24.55	C
ATOM	473	CB	MET	A	390	-3.353	-12.085	-6.809	1.00	24.16	C
ATOM	474	CG	MET	A	390	-2.457	-11.523	-5.714	1.00	24.68	C
ATOM	475	SD	MET	A	390	-0.694	-11.770	-6.180	1.00	31.52	S
ATOM	476	CE	MET	A	390	-0.450	-10.325	-7.210	1.00	31.50	C
ATOM	477	C	MET	A	390	-5.638	-12.215	-7.807	1.00	29.46	C
ATOM	478	O	MET	A	390	-5.960	-11.302	-8.558	1.00	30.11	O
ATOM	479	N	HIS	A	391	-5.945	-13.493	-8.024	1.00	30.83	N
ATOM	480	CA	HIS	A	391	-6.689	-13.890	-9.230	1.00	37.84	C
ATOM	481	CB	HIS	A	391	-6.738	-15.420	-9.340	1.00	43.52	C
ATOM	482	CG	HIS	A	391	-7.283	-15.921	-10.645	1.00	49.94	C
ATOM	483	CD2	HIS	A	391	-6.657	-16.380	-11.756	1.00	51.86	C
ATOM	484	ND1	HIS	A	391	-8.633	-15.956	-10.924	1.00	55.85	N
ATOM	485	CE1	HIS	A	391	-8.816	-16.416	-12.149	1.00	57.35	C
ATOM	486	NE2	HIS	A	391	-7.634	-16.681	-12.675	1.00	57.80	N
ATOM	487	C	HIS	A	391	-8.106	-13.321	-9.231	1.00	42.10	C
ATOM	488	O	HIS	A	391	-8.778	-13.315	-10.262	1.00	47.79	O
ATOM	489	N	GLN	A	392	-8.559	-12.839	-8.077	1.00	39.91	N
ATOM	490	CA	GLN	A	392	-9.898	-12.259	-7.965	1.00	41.34	C
ATOM	491	CB	GLN	A	392	-10.543	-12.659	-6.633	1.00	43.83	C
ATOM	492	CG	GLN	A	392	-10.631	-14.161	-6.437	1.00	47.90	C
ATOM	493	CD	GLN	A	392	-11.399	-14.548	-5.197	1.00	51.89	C
ATOM	494	OE1	GLN	A	392	-12.612	-14.361	-5.124	1.00	58.95	O
ATOM	495	NE2	GLN	A	392	-10.699	-15.095	-4.210	1.00	51.91	N
ATOM	496	C	GLN	A	392	-9.860	-10.742	-8.067	1.00	46.24	C
ATOM	497	O	GLN	A	392	-10.888	-10.081	-7.932	1.00	43.30	O
ATOM	498	N	LEU	A	393	-8.676	-10.190	-8.317	1.00	43.90	N
ATOM	499	CA	LEU	A	393	-8.511	-8.741	-8.416	1.00	43.71	C
ATOM	500	CB	LEU	A	393	-7.350	-8.287	-7.530	1.00	46.31	C
ATOM	501	CG	LEU	A	393	-7.356	-8.772	-6.080	1.00	47.53	C
ATOM	502	CD1	LEU	A	393	-6.097	-8.274	-5.384	1.00	44.78	C
ATOM	503	CD2	LEU	A	393	-8.601	-8.278	-5.364	1.00	38.33	C
ATOM	504	C	LEU	A	393	-8.269	-8.257	-9.843	1.00	45.51	C
ATOM	505	O	LEU	A	393	-7.485	-8.847	-10.597	1.00	50.21	O

ATOM	506	N	ASP	A	394	-8.924	-7.167	-10.220	1.00	41.60	N
ATOM	507	CA	ASP	A	394	-8.759	-6.638	-11.565	1.00	38.62	C
ATOM	508	CB	ASP	A	394	-9.874	-7.175	-12.473	1.00	45.48	C
ATOM	509	CG	ASP	A	394	-9.733	-6.718	-13.917	1.00	53.93	C
ATOM	510	OD1	ASP	A	394	-10.609	-7.075	-14.740	1.00	54.65	O
ATOM	511	OD2	ASP	A	394	-8.756	-6.009	-14.235	1.00	49.40	O
ATOM	512	C	ASP	A	394	-8.821	-5.132	-11.499	1.00	41.64	C
ATOM	513	O	ASP	A	394	-9.870	-4.523	-11.744	1.00	41.10	O
ATOM	514	N	ASN	A	395	-7.692	-4.519	-11.169	1.00	38.06	N
ATOM	515	CA	ASN	A	395	-7.654	-3.075	-11.057	1.00	29.93	C
ATOM	516	CB	ASN	A	395	-7.902	-2.678	-9.592	1.00	27.46	C
ATOM	517	CG	ASN	A	395	-8.027	-1.187	-9.397	1.00	34.86	C
ATOM	518	OD1	ASN	A	395	-9.106	-0.602	-9.581	1.00	38.20	O
ATOM	519	ND2	ASN	A	395	-6.923	-0.552	-9.025	1.00	25.87	N
ATOM	520	C	ASN	A	395	-6.285	-2.610	-11.530	1.00	30.95	C
ATOM	521	O	ASN	A	395	-5.258	-3.260	-11.269	1.00	28.17	O
ATOM	522	N	PRO	A	396	-6.248	-1.467	-12.222	1.00	28.97	N
ATOM	523	CD	PRO	A	396	-7.395	-0.706	-12.748	1.00	39.56	C
ATOM	524	CA	PRO	A	396	-4.996	-0.919	-12.733	1.00	28.79	C
ATOM	525	CB	PRO	A	396	-5.464	0.277	-13.556	1.00	37.29	C
ATOM	526	CG	PRO	A	396	-6.842	-0.149	-14.019	1.00	42.13	C
ATOM	527	C	PRO	A	396	-3.997	-0.494	-11.656	1.00	28.11	C
ATOM	528	O	PRO	A	396	-2.821	-0.352	-11.939	1.00	27.45	O
ATOM	529	N	TYR	A	397	-4.471	-0.298	-10.422	1.00	24.07	N
ATOM	530	CA	TYR	A	397	-3.576	0.171	-9.346	1.00	22.72	C
ATOM	531	CB	TYR	A	397	-4.250	1.346	-8.618	1.00	21.97	C
ATOM	532	CG	TYR	A	397	-4.655	2.442	-9.593	1.00	25.66	C
ATOM	533	CD1	TYR	A	397	-5.994	2.640	-9.946	1.00	29.62	C
ATOM	534	CE1	TYR	A	397	-6.356	3.604	-10.886	1.00	34.32	C
ATOM	535	CD2	TYR	A	397	-3.689	3.238	-10.206	1.00	25.78	C
ATOM	536	CE2	TYR	A	397	-4.044	4.206	-11.152	1.00	36.01	C
ATOM	537	CZ	TYR	A	397	-5.376	4.380	-11.490	1.00	37.11	C
ATOM	538	OH	TYR	A	397	-5.694	5.301	-12.473	1.00	40.47	O
ATOM	539	C	TYR	A	397	-3.127	-0.896	-8.368	1.00	21.63	C
ATOM	540	O	TYR	A	397	-2.730	-0.615	-7.213	1.00	23.29	O
ATOM	541	N	ILE	A	398	-3.193	-2.125	-8.832	1.00	22.86	N
ATOM	542	CA	ILE	A	398	-2.770	-3.266	-8.069	1.00	29.14	C
ATOM	543	CB	ILE	A	398	-4.005	-4.065	-7.641	1.00	34.44	C
ATOM	544	CG2	ILE	A	398	-3.602	-5.424	-7.156	1.00	37.06	C
ATOM	545	CG1	ILE	A	398	-4.768	-3.273	-6.575	1.00	28.40	C
ATOM	546	CD1	ILE	A	398	-6.166	-3.759	-6.305	1.00	41.40	C
ATOM	547	C	ILE	A	398	-1.858	-4.102	-8.975	1.00	33.99	C
ATOM	548	O	ILE	A	398	-2.096	-4.193	-10.183	1.00	34.40	O
ATOM	549	N	VAL	A	399	-0.805	-4.672	-8.402	1.00	27.19	N
ATOM	550	CA	VAL	A	399	0.109	-5.540	-9.155	1.00	26.99	C
ATOM	551	CB	VAL	A	399	1.298	-6.006	-8.302	1.00	29.43	C
ATOM	552	CG1	VAL	A	399	2.078	-7.146	-9.026	1.00	26.20	C
ATOM	553	CG2	VAL	A	399	2.200	-4.832	-8.031	1.00	30.03	C
ATOM	554	C	VAL	A	399	-0.704	-6.759	-9.539	1.00	33.87	C
ATOM	555	O	VAL	A	399	-1.162	-7.498	-8.670	1.00	35.03	O
ATOM	556	N	ARG	A	400	-0.849	-6.986	-10.837	1.00	26.00	N
ATOM	557	CA	ARG	A	400	-1.652	-8.098	-11.315	1.00	30.60	C
ATOM	558	CB	ARG	A	400	-2.172	-7.785	-12.728	1.00	38.54	C
ATOM	559	CG	ARG	A	400	-3.035	-6.521	-12.854	1.00	46.40	C
ATOM	560	CD	ARG	A	400	-3.410	-6.240	-14.331	1.00	46.44	C
ATOM	561	NE	ARG	A	400	-4.269	-5.066	-14.505	1.00	52.85	N
ATOM	562	CZ	ARG	A	400	-5.554	-5.032	-14.163	1.00	56.01	C
ATOM	563	NH1	ARG	A	400	-6.117	-6.110	-13.633	1.00	52.93	N
ATOM	564	NH2	ARG	A	400	-6.276	-3.928	-14.346	1.00	53.59	N
ATOM	565	C	ARG	A	400	-0.946	-9.444	-11.324	1.00	27.57	C
ATOM	566	O	ARG	A	400	0.257	-9.548	-11.572	1.00	27.90	O
ATOM	567	N	LEU	A	401	-1.703	-10.500	-11.077	1.00	28.32	N
ATOM	568	CA	LEU	A	401	-1.147	-11.838	-11.096	1.00	24.81	C
ATOM	569	CB	LEU	A	401	-1.974	-12.777	-10.238	1.00	32.19	C
ATOM	570	CG	LEU	A	401	-1.534	-14.239	-10.271	1.00	29.13	C
ATOM	571	CD1	LEU	A	401	-0.159	-14.414	-9.638	1.00	37.61	C
ATOM	572	CD2	LEU	A	401	-2.578	-15.046	-9.516	1.00	42.15	C
ATOM	573	C	LEU	A	401	-1.194	-12.352	-12.525	1.00	32.86	C

ATOM	574	O	LEU	A	401	-2.248	-12.281	-13.176	1.00	30.25	O
ATOM	575	N	ILE	A	402	-0.060	-12.831	-13.026	1.00	26.16	N
ATOM	576	CA	ILE	A	402	-0.031	-13.405	-14.364	1.00	28.41	C
ATOM	577	CB	ILE	A	402	1.394	-13.397	-14.987	1.00	29.05	C
ATOM	578	CG2	ILE	A	402	1.360	-14.080	-16.360	1.00	33.43	C
ATOM	579	CG1	ILE	A	402	1.898	-11.957	-15.135	1.00	28.86	C
ATOM	580	CD1	ILE	A	402	0.925	-11.026	-15.810	1.00	33.60	C
ATOM	581	C	ILE	A	402	-0.508	-14.853	-14.187	1.00	31.32	C
ATOM	582	O	ILE	A	402	-1.402	-15.330	-14.890	1.00	29.93	O
ATOM	583	N	GLY	A	403	0.070	-15.548	-13.224	1.00	29.11	N
ATOM	584	CA	GLY	A	403	-0.335	-16.924	-12.971	1.00	28.71	C
ATOM	585	C	GLY	A	403	0.639	-17.626	-12.060	1.00	29.89	C
ATOM	586	O	GLY	A	403	1.605	-17.020	-11.612	1.00	29.79	O
ATOM	587	N	VAL	A	404	0.387	-18.900	-11.787	1.00	27.61	N
ATOM	588	CA	VAL	A	404	1.259	-19.697	-10.938	1.00	31.08	C
ATOM	589	CB	VAL	A	404	0.436	-20.508	-9.911	1.00	36.46	C
ATOM	590	CG1	VAL	A	404	1.360	-21.378	-9.052	1.00	42.77	C
ATOM	591	CG2	VAL	A	404	-0.370	-19.564	-9.051	1.00	37.69	C
ATOM	592	C	VAL	A	404	2.019	-20.671	-11.823	1.00	29.99	C
ATOM	593	O	VAL	A	404	1.480	-21.154	-12.802	1.00	32.94	O
ATOM	594	N	CYS	A	405	3.262	-20.969	-11.461	1.00	31.70	N
ATOM	595	CA	CYS	A	405	4.065	-21.908	-12.243	1.00	37.20	C
ATOM	596	CB	CYS	A	405	5.131	-21.150	-13.042	1.00	40.22	C
ATOM	597	SG	CYS	A	405	5.968	-22.154	-14.282	1.00	46.07	S
ATOM	598	C	CYS	A	405	4.717	-22.939	-11.324	1.00	40.66	C
ATOM	599	O	CYS	A	405	5.428	-22.587	-10.388	1.00	39.23	O
ATOM	600	N	GLN	A	406	4.453	-24.213	-11.583	1.00	40.69	N
ATOM	601	CA	GLN	A	406	5.011	-25.282	-10.762	1.00	50.34	C
ATOM.	602	CB	GLN	A	406	3.900	-26.245	-10.326	1.00	53.46	C
ATOM	603	CG	GLN	A	406	4.373	-27.437	-9.486	1.00	59.61	C
ATOM	604	CD	GLN	A	406	5.156	-27.032	-8.240	1.00	55.65	C
ATOM	605	OE1	GLN	A	406	6.329	-26.665	-8.316	1.00	61.62	O
ATOM	606	NE2	GLN	A	406	4.504	-27.099	-7.088	1.00	58.42	N
ATOM	607	C	GLN	A	406	6.090	-26.044	-11.519	1.00	53.49	C
ATOM	608	O	GLN	A	406	5.792	-26.902	-12.345	1.00	56.41	O
ATOM	609	N	ALA	A	407	7.342	-25.718	-11.234	1.00	54.94	N
ATOM	610	CA	ALA	A	407	8.468	-26.378	-11.879	1.00	59.69	C
ATOM	611	CB	ALA	A	407	9.105	-25.437	-12.902	1.00	59.62	C
ATOM	612	C	ALA	A	407	9.484	-26.782	-10.811	1.00	57.77	C
ATOM	613	O	ALA	A	407	9.173	-27.578	-9.923	1.00	57.65	O
ATOM	614	N	GLU	A	408	10.692	-26.232	-10.895	1.00	54.86	N
ATOM	615	CA	GLU	A	408	11.730	-26.541	-9.921	1.00	56.21	C
ATOM	616	CB	GLU	A	408	13.002	-25.738	-10.220	1.00	60.73	C
ATOM	617	CG	GLU	A	408	12.777	-24.237	-10.370	1.00	60.37	C
ATOM	618	CD	GLU	A	408	12.597	-23.801	-11.818	1.00	61.95	C
ATOM	619	OE1	GLU	A	408	11.749	-24.377	-12.535	1.00	61.59	O
ATOM	620	OE2	GLU	A	408	13.308	-22.866	-12.238	1.00	60.74	O
ATOM	621	C	GLU	A	408	11.216	-26.210	-8.524	1.00	57.49	C
ATOM	622	O	GLU	A	408	11.766	-26.663	-7.517	1.00	60.01	O
ATOM	623	N	ALA	A	409	10.155	-25.411	-8.480	1.00	56.44	N
ATOM	624	CA	ALA	A	409	9.519	-25.007	-7.231	1.00	52.91	C
ATOM	625	CB	ALA	A	409	10.480	-24.178	-6.392	1.00	58.00	C
ATOM	626	C	ALA	A	409	8.276	-24.196	-7.589	1.00	49.70	C
ATOM	627	O	ALA	A	409	8.092	-23.822	-8.750	1.00	46.56	O
ATOM	628	N	LEU	A	410	7.420	-23.942	-6.601	1.00	48.39	N
ATOM	629	CA	LEU	A	410	6.189	-23.192	-6.830	1.00	42.60	C
ATOM	630	CB	LEU	A	410	5.210	-23.433	-5.681	1.00	42.05	C
ATOM	631	CG	LEU	A	410	3.794	-22.949	-5.968	1.00	39.06	C
ATOM	632	CD1	LEU	A	410	3.256	-23.669	-7.199	1.00	42.72	C
ATOM	633	CD2	LEU	A	410	2.912	-23.207	-4.752	1.00	46.20	C
ATOM	634	C	LEU	A	410	6.516	-21.711	-6.941	1.00	34.88	C
ATOM	635	O	LEU	A	410	7.246	-21.174	-6.118	1.00	32.97	O
ATOM	636	N	MET	A	411	5.969	-21.052	-7.956	1.00	32.78	N
ATOM	637	CA	MET	A	411	6.269	-19.647	-8.171	1.00	27.80	C
ATOM	638	CB	MET	A	411	7.272	-19.506	-9.326	1.00	29.67	C
ATOM	639	CG	MET	A	411	8.546	-20.333	-9.200	1.00	37.85	C
ATOM	640	SD	MET	A	411	9.647	-20.153	-10.644	1.00	40.33	S
ATOM	641	CE	MET	A	411	8.672	-20.909	-11.859	1.00	38.19	C

ATOM	642	C	MET	A	411	5.024	-18.846	-8.521	1.00	29.61	C
ATOM	643	O	MET	A	411	4.126	-19.354	-9.171	1.00	32.53	O
ATOM	644	N	LEU	A	412	4.975	-17.593	-8.083	1.00	26.11	N
ATOM	645	CA	LEU	A	412	3.864	-16.704	-8.426	1.00	23.60	C
ATOM	646	CB	LEU	A	412	3.340	-15.957	-7.197	1.00	30.66	C
ATOM	647	CG	LEU	A	412	2.475	-16.741	-6.224	1.00	43.14	C
ATOM	648	CD1	LEU	A	412	1.856	-15.774	-5.208	1.00	39.76	C
ATOM	649	CD2	LEU	A	412	1.389	-17.457	-7.018	1.00	42.58	C
ATOM	650	C	LEU	A	412	4.450	-15.688	-9.391	1.00	33.31	C
ATOM	651	O	LEU	A	412	5.348	-14.947	-9.004	1.00	24.93	O
ATOM	652	N	VAL	A	413	3.928	-15.663	-10.626	1.00	26.19	N
ATOM	653	CA	VAL	A	413	4.385	-14.739	-11.674	1.00	24.01	C
ATOM	654	CB	VAL	A	413	4.374	-15.425	-13.070	1.00	25.63	C
ATOM	655	CG1	VAL	A	413	4.951	-14.465	-14.143	1.00	22.85	C
ATOM	656	CG2	VAL	A	413	5.192	-16.718	-13.010	1.00	26.67	C
ATOM	657	C	VAL	A	413	3.458	-13.540	-11.700	1.00	26.19	C
ATOM	658	O	VAL	A	413	2.240	-13.673	-11.925	1.00	28.56	O
ATOM	659	N	MET	A	414	4.052	-12.368	-11.490	1.00	22.49	N
ATOM	660	CA	MET	A	414	3.324	-11.108	-11.418	1.00	22.14	C
ATOM	661	CB	MET	A	414	3.422	-10.545	-9.987	1.00	25.30	C
ATOM	662	CG	MET	A	414	2.767	-11.409	-8.917	1.00	28.88	C
ATOM	663	SD	MET	A	414	3.377	-10.874	-7.264	1.00	30.85	S
ATOM	664	CE	MET	A	414	4.890	-11.872	-7.109	1.00	32.45	C
ATOM	665	C	MET	A	414	3.871	-10.049	-12.336	1.00	24.63	C
ATOM	666	O	MET	A	414	5.017	-10.131	-12.796	1.00	25.46	O
ATOM	667	N	GLU	A	415	3.075	-9.012	-12.568	1.00	25.97	N
ATOM	668	CA	GLU	A	415	3.548	-7.913	-13.395	1.00	25.91	C
ATOM	669	CB	GLU	A	415	2.470	-6.842	-13.568	1.00	37.31	C
ATOM	670	CG	GLU	A	415	1.181	-7.321	-14.191	1.00	41.51	C
ATOM	671	CD	GLU	A	415	0.151	-6.190	-14.258	1.00	56.50	C
ATOM	672	OE1	GLU	A	415	-0.056	-5.493	-13.222	1.00	39.84	O
ATOM	673	OE2	GLU	A	415	-0.444	-5.998	-15.346	1.00	55.15	O
ATOM	674	C	GLU	A	415	4.711	-7.273	-12.651	1.00	26.45	C
ATOM	675	O	GLU	A	415	4.751	-7.287	-11.417	1.00	26.92	O
ATOM	676	N	MET	A	416	5.657	-6.713	-13.400	1.00	27.12	N
ATOM	677	CA	MET	A	416	6.784	-6.047	-12.778	1.00	26.18	C
ATOM	678	CB	MET	A	416	8.078	-6.343	-13.519	1.00	29.98	C
ATOM	679	CG	MET	A	416	9.308	-5.885	-12.729	1.00	32.43	C
ATOM	680	SD	MET	A	416	10.835	-6.141	-13.631	1.00	40.73	S
ATOM	681	CE	MET	A	416	11.931	-4.939	-12.809	1.00	40.48	C
ATOM	682	C	MET	A	416	6.577	-4.539	-12.781	1.00	30.68	C
ATOM	683	O	MET	A	416	6.117	-3.981	-13.766	1.00	29.07	O
ATOM	684	N	ALA	A	417	6.916	-3.893	-11.670	1.00	28.26	N
ATOM	685	CA	ALA	A	417	6.843	-2.436	-11.561	1.00	31.40	C
ATOM	686	CB	ALA	A	417	5.886	-2.019	-10.435	1.00	31.37	C
ATOM	687	C	ALA	A	417	8.286	-2.023	-11.253	1.00	31.10	C
ATOM	688	O	ALA	A	417	8.672	-1.865	-10.087	1.00	31.97	O
ATOM	689	N	GLY	A	418	9.064	-1.876	-12.330	1.00	35.10	N
ATOM	690	CA	GLY	A	418	10.485	-1.554	-12.258	1.00	34.74	C
ATOM	691	C	GLY	A	418	10.936	-0.340	-11.474	1.00	32.22	C
ATOM	692	O	GLY	A	418	12.120	-0.205	-11.147	1.00	33.36	O
ATOM	693	N	GLY	A	419	10.002	0.559	-11.183	1.00	26.94	N
ATOM	694	CA	GLY	A	419	10.354	1.740	-10.421	1.00	27.31	C
ATOM	695	C	GLY	A	419	10.674	1.386	-8.978	1.00	32.93	C
ATOM	696	O	GLY	A	419	11.321	2.150	-8.287	1.00	31.61	O
ATOM	697	N	GLY	A	420	10.196	0.235	-8.506	1.00	32.29	N
ATOM	698	CA	GLY	A	420	10.469	-0.166	-7.139	1.00	27.34	C
ATOM	699	C	GLY	A	420	9.632	0.511	-6.054	1.00	27.22	C
ATOM	700	O	GLY	A	420	8.709	1.263	-6.369	1.00	25.34	O
ATOM	701	N	PRO	A	421	9.952	0.280	-4.770	1.00	27.85	N
ATOM	702	CD	PRO	A	421	11.122	-0.509	-4.330	1.00	29.71	C
ATOM	703	CA	PRO	A	421	9.247	0.843	-3.612	1.00	25.99	C
ATOM	704	CB	PRO	A	421	10.049	0.310	-2.411	1.00	33.47	C
ATOM	705	CG	PRO	A	421	10.755	-0.872	-2.921	1.00	33.83	C
ATOM	706	C	PRO	A	421	9.178	2.358	-3.574	1.00	32.23	C
ATOM	707	O	PRO	A	421	10.162	3.052	-3.845	1.00	25.70	O
ATOM	708	N	LEU	A	422	8.002	2.856	-3.196	1.00	24.75	N
ATOM	709	CA	LEU	A	422	7.726	4.280	-3.094	1.00	24.74	C

ATOM	710	CB	LEU	A	422	6.258	4.475	-2.705	1.00	25.86	C
ATOM	711	CG	LEU	A	422	5.736	5.899	-2.536	1.00	27.46	C
ATOM	712	CD1	LEU	A	422	5.749	6.599	-3.879	1.00	29.48	C
ATOM	713	CD2	LEU	A	422	4.322	5.851	-1.989	1.00	26.17	C
ATOM	714	C	LEU	A	422	8.607	5.010	-2.078	1.00	24.09	C
ATOM	715	O	LEU	A	422	9.065	6.128	-2.347	1.00	27.09	O
ATOM	716	N	HIS	A	423	8.821	4.423	-0.908	1.00	23.84	N
ATOM	717	CA	HIS	A	423	9.627	5.097	0.097	1.00	31.59	C
ATOM	718	CB	HIS	A	423	9.677	4.309	1.410	1.00	33.34	C
ATOM	719	CG	HIS	A	423	10.255	2.935	1.274	1.00	32.56	C
ATOM	720	CD2	HIS	A	423	10.263	2.066	0.236	1.00	33.97	C
ATOM	721	ND1	HIS	A	423	10.947	2.318	2.296	1.00	40.55	N
ATOM	722	CE1	HIS	A	423	11.355	1.128	1.894	1.00	33.85	C
ATOM	723	NE2	HIS	A	423	10.952	0.950	0.647	1.00	37.19	N
ATOM	724	C	HIS	A	423	11.048	5.352	-0.417	1.00	35.72	C
ATOM	725	O	HIS	A	423	11.583	6.444	-0.235	1.00	38.98	O
ATOM	726	N	LYS	A	424	11.647	4.356	-1.064	1.00	26.67	N
ATOM	727	CA	LYS	A	424	13.000	4.559	-1.576	1.00	30.40	C
ATOM	728	CB	LYS	A	424	13.625	3.217	-1.950	1.00	30.75	C
ATOM	729	CG	LYS	A	424	13.884	2.327	-0.747	1.00	32.42	C
ATOM	730	CD	LYS	A	424	14.486	0.996	-1.191	1.00	42.37	C
ATOM	731	CE	LYS	A	424	14.635	0.035	-0.020	1.00	47.25	C
ATOM	732	NZ	LYS	A	424	15.606	-1.054	-0.360	1.00	54.40	N
ATOM	733	C	LYS	A	424	13.025	5.500	-2.767	1.00	30.87	C
ATOM	734	O	LYS	A	424	13.976	6.259	-2.944	1.00	27.95	O
ATOM	735	N	PHE	A	425	11.975	5.479	-3.586	1.00	27.56	N
ATOM	736	CA	PHE	A	425	11.919	6.345	-4.755	1.00	27.56	C
ATOM	737	CB	PHE	A	425	10.693	6.006	-5.612	1.00	33.85	C
ATOM	738	CG	PHE	A	425	10.536	6.885	-6.816	1.00	33.08	C
ATOM	739	CD1	PHE	A	425	11.259	6.634	-7.976	1.00	43.47	C
ATOM	740	CD2	PHE	A	425	9.692	7.986	-6.778	1.00	38.10	C
ATOM	741	CE1	PHE	A	425	11.146	7.473	-9.083	1.00	42.11	C
ATOM	742	CE2	PHE	A	425	9.567	8.832	-7.874	1.00	47.88	C
ATOM	743	CZ	PHE	A	425	10.297	8.574	-9.033	1.00	44.70	C
ATOM	744	C	PHE	A	425	11.861	7.838	-4.391	1.00	29.42	C
ATOM	745	O	PHE	A	425	12.421	8.681	-5.097	1.00	28.17	O
ATOM	746	N	LEU	A	426	11.198	8.174	-3.295	1.00	26.78	N
ATOM	747	CA	LEU	A	426	11.053	9.581	-2.919	1.00	23.65	C
ATOM	748	CB	LEU	A	426	9.750	9.793	-2.142	1.00	23.99	C
ATOM	749	CG	LEU	A	426	8.484	9.534	-2.972	1.00	23.37	C
ATOM	750	CD1	LEU	A	426	7.234	9.646	-2.081	1.00	23.77	C
ATOM	751	CD2	LEU	A	426	8.429	10.547	-4.096	1.00	27.33	C
ATOM	752	C	LEU	A	426	12.210	10.161	-2.100	1.00	29.71	C
ATOM	753	O	LEU	A	426	12.345	11.379	-2.011	1.00	24.55	O
ATOM	754	N	VAL	A	427	13.021	9.296	-1.501	1.00	25.47	N
ATOM	755	CA	VAL	A	427	14.130	9.781	-0.661	1.00	28.99	C
ATOM	756	CB	VAL	A	427	14.996	8.607	-0.132	1.00	34.76	C
ATOM	757	CG1	VAL	A	427	16.250	9.148	0.578	1.00	37.93	C
ATOM	758	CG2	VAL	A	427	14.186	7.762	0.852	1.00	30.76	C
ATOM	759	C	VAL	A	427	15.027	10.780	-1.403	1.00	34.84	C
ATOM	760	O	VAL	A	427	15.605	10.464	-2.445	1.00	37.55	O
ATOM	761	N	GLY	A	428	15.117	11.993	-0.862	1.00	43.08	N
ATOM	762	CA	GLY	A	428	15.941	13.030	-1.469	1.00	41.65	C
ATOM	763	C	GLY	A	428	15.437	13.634	-2.768	1.00	47.74	C
ATOM	764	O	GLY	A	428	16.196	14.303	-3.479	1.00	42.77	O
ATOM	765	N	LYS	A	429	14.163	13.430	-3.090	1.00	37.30	N
ATOM	766	CA	LYS	A	429	13.624	13.972	-4.328	1.00	41.14	C
ATOM	767	CB	LYS	A	429	13.024	12.840	-5.161	1.00	46.03	C
ATOM	768	CG	LYS	A	429	14.064	11.799	-5.568	1.00	46.82	C
ATOM	769	CD	LYS	A	429	13.607	11.007	-6.775	1.00	54.33	C
ATOM	770	CE	LYS	A	429	14.575	9.879	-7.099	1.00	52.59	C
ATOM	771	NZ	LYS	A	429	14.028	9.018	-8.182	1.00	61.02	N
ATOM	772	C	LYS	A	429	12.596	15.079	-4.098	1.00	43.46	C
ATOM	773	O	LYS	A	429	11.741	15.347	-4.952	1.00	46.64	O
ATOM	774	N	ARG	A	430	12.696	15.736	-2.950	1.00	38.34	N
ATOM	775	CA	ARG	A	430	11.765	16.798	-2.604	1.00	51.71	C
ATOM	776	CB	ARG	A	430	12.050	17.298	-1.189	1.00	53.36	C
ATOM	777	CG	ARG	A	430	10.922	18.125	-0.591	1.00	62.96	C

ATOM	778	CD	ARG	A	430	11.039	18.217	0.928	1.00	63.14	C
ATOM	779	NE	ARG	A	430	9.729	18.100	1.576	1.00	62.24	N
ATOM	780	CZ	ARG	A	430	9.526	17.461	2.724	1.00	68.34	C
ATOM	781	NH1	ARG	A	430	10.545	16.890	3.355	1.00	63.91	N
ATOM	782	NH2	ARG	A	430	8.293	17.358	3.231	1.00	65.90	N
ATOM	783	C	ARG	A	430	11.818	17.957	-3.591	1.00	54.65	C
ATOM	784	O	ARG	A	430	10.867	18.723	-3.716	1.00	53.09	O
ATOM	785	N	GLU	A	431	12.932	18.078	-4.307	1.00	55.81	N
ATOM	786	CA	GLU	A	431	13.077	19.158	-5.268	1.00	54.84	C
ATOM	787	CB	GLU	A	431	14.428	19.855	-5.092	1.00	58.53	C
ATOM	788	CG	GLU	A	431	14.491	20.755	-3.869	1.00	61.42	C
ATOM	789	CD	GLU	A	431	15.662	21.716	-3.910	1.00	67.37	C
ATOM	790	OE1	GLU	A	431	15.715	22.555	-4.841	1.00	71.67	O
ATOM	791	OE2	GLU	A	431	16.530	21.638	-3.013	1.00	68.85	O
ATOM	792	C	GLU	A	431	12.913	18.709	-6.705	1.00	55.28	C
ATOM	793	O	GLU	A	431	12.995	19.521	-7.622	1.00	58.15	O
ATOM	794	N	GLU	A	432	12.678	17.420	-6.912	1.00	50.44	N
ATOM	795	CA	GLU	A	432	12.498	16.923	-8.263	1.00	48.35	C
ATOM	796	CB	GLU	A	432	13.596	15.918	-8.623	1.00	55.95	C
ATOM	797	CG	GLU	A	432	13.285	14.477	-8.287	1.00	59.72	C
ATOM	798	CD	GLU	A	432	14.264	13.513	-8.934	1.00	62.60	C
ATOM	799	OE1	GLU	A	432	15.463	13.571	-8.594	1.00	66.37	O
ATOM	800	OE2	GLU	A	432	13.837	12.700	-9.786	1.00	65.64	O
ATOM	801	C	GLU	A	432	11.125	16.285	-8.432	1.00	47.94	C
ATOM	802	O	GLU	A	432	10.661	16.082	-9.548	1.00	47.37	O
ATOM	803	N	ILE	A	433	10.474	15.968	-7.315	1.00	39.35	N
ATOM	804	CA	ILE	A	433	9.143	15.364	-7.361	1.00	35.26	C
ATOM	805	CB	ILE	A	433	9.148	13.942	-6.758	1.00	40.43	C
ATOM	806	CG2	ILE	A	433	7.742	13.332	-6.819	1.00	32.65	C
ATOM	807	CG1	ILE	A	433	10.120	13.056	-7.527	1.00	39.75	C
ATOM	808	CD1	ILE	A	433	9.720	12.837	-8.964	1.00	41.51	C
ATOM	809	C	ILE	A	433	8.252	16.258	-6.521	1.00	36.84	C
ATOM	810	O	ILE	A	433	8.276	16.182	-5.291	1.00	32.85	O
ATOM	811	N	PRO	A	434	7.467	17.134	-7.172	1.00	33.02	N
ATOM	812	CD	PRO	A	434	7.510	17.400	-8.618	1.00	41.68	C
ATOM	813	CA	PRO	A	434	6.554	18.074	-6.512	1.00	36.57	C
ATOM	814	CB	PRO	A	434	5.925	18.812	-7.693	1.00	37.02	C
ATOM	815	CG	PRO	A	434	7.033	18.833	-8.679	1.00	47.39	C
ATOM	816	C	PRO	A	434	5.512	17.377	-5.648	1.00	31.45	C
ATOM	817	O	PRO	A	434	5.227	16.199	-5.848	1.00	28.84	O
ATOM	818	N	VAL	A	435	4.944	18.121	-4.702	1.00	32.88	N
ATOM	819	CA	VAL	A	435	3.919	17.568	-3.821	1.00	34.12	C
ATOM	820	CB	VAL	A	435	3.457	18.619	-2.777	1.00	32.16	C
ATOM	821	CG1	VAL	A	435	2.335	18.041	-1.904	1.00	32.92	C
ATOM	822	CG2	VAL	A	435	4.629	19.012	-1.901	1.00	39.50	C
ATOM	823	C	VAL	A	435	2.731	17.093	-4.642	1.00	34.03	C
ATOM	824	O	VAL	A	435	2.096	16.076	-4.299	1.00	26.73	O
ATOM	825	N	SER	A	436	2.424	17.821	-5.721	1.00	27.34	N
ATOM	826	CA	SER	A	436	1.321	17.445	-6.595	1.00	26.52	C
ATOM	827	CB	SER	A	436	1.152	18.482	-7.725	1.00	34.16	C
ATOM	828	OG	SER	A	436	2.339	18.588	-8.494	1.00	36.95	O
ATOM	829	C	SER	A	436	1.517	16.038	-7.187	1.00	29.26	C
ATOM	830	O	SER	A	436	0.548	15.298	-7.359	1.00	28.55	O
ATOM	831	N	ASN	A	437	2.763	15.676	-7.486	1.00	24.99	N
ATOM	832	CA	ASN	A	437	3.085	14.372	-8.060	1.00	24.95	C
ATOM	833	CB	ASN	A	437	4.499	14.432	-8.649	1.00	30.76	C
ATOM	834	CG	ASN	A	437	4.891	13.192	-9.462	1.00	33.40	C
ATOM	835	OD1	ASN	A	437	5.922	13.209	-10.140	1.00	31.35	O
ATOM	836	ND2	ASN	A	437	4.107	12.116	-9.381	1.00	33.64	N
ATOM	837	C	ASN	A	437	2.957	13.330	-6.923	1.00	24.92	C
ATOM	838	O	ASN	A	437	2.472	12.224	-7.133	1.00	26.65	O
ATOM	839	N	VAL	A	438	3.371	13.695	-5.719	1.00	25.75	N
ATOM	840	CA	VAL	A	438	3.201	12.755	-4.612	1.00	24.63	C
ATOM	841	CB	VAL	A	438	3.819	13.291	-3.321	1.00	28.75	C
ATOM	842	CG1	VAL	A	438	3.496	12.348	-2.162	1.00	25.61	C
ATOM	843	CG2	VAL	A	438	5.338	13.426	-3.500	1.00	27.56	C
ATOM	844	C	VAL	A	438	1.697	12.523	-4.409	1.00	24.68	C
ATOM	845	O	VAL	A	438	1.277	11.391	-4.258	1.00	22.54	O

ATOM	846	N	ALA	A	439	0.888	13.591	-4.441	1.00	22.86	N
ATOM	847	CA	ALA	A	439	-0.567	13.437	-4.280	1.00	25.85	C
ATOM	848	CB	ALA	A	439	-1.263	14.843	-4.217	1.00	25.16	C
ATOM	849	C	ALA	A	439	-1.188	12.589	-5.395	1.00	22.87	C
ATOM	850	O	ALA	A	439	-2.146	11.861	-5.154	1.00	23.17	O
ATOM	851	N	GLU	A	440	-0.647	12.685	-6.614	1.00	21.21	N
ATOM	852	CA	GLU	A	440	-1.157	11.900	-7.728	1.00	25.32	C
ATOM	853	CB	GLU	A	440	-0.380	12.246	-9.014	1.00	30.55	C
ATOM	854	CG	GLU	A	440	-0.636	11.301	-10.184	1.00	29.05	C
ATOM	855	CD	GLU	A	440	0.286	11.582	-11.368	1.00	40.39	C
ATOM	856	OE1	GLU	A	440	1.448	11.984	-11.145	1.00	35.18	O
ATOM	857	OE2	GLU	A	440	-0.151	11.385	-12.523	1.00	36.07	O
ATOM	858	C	GLU	A	440	-0.998	10.404	-7.406	1.00	31.15	C
ATOM	859	O	GLU	A	440	-1.923	9.614	-7.585	1.00	23.98	O
ATOM	860	N	LEU	A	441	0.181	10.035	-6.913	1.00	24.24	N
ATOM	861	CA	LEU	A	441	0.500	8.646	-6.573	1.00	21.78	C
ATOM	862	CB	LEU	A	441	1.991	8.541	-6.222	1.00	22.41	C
ATOM	863	CG	LEU	A	441	2.937	8.916	-7.366	1.00	22.95	C
ATOM	864	CD1	LEU	A	441	4.389	8.882	-6.901	1.00	27.25	C
ATOM	865	CD2	LEU	A	441	2.720	7.939	-8.521	1.00	19.84	C
ATOM	866	C	LEU	A	441	-0.354	8.186	-5.377	1.00	18.04	C
ATOM	867	O	LEU	A	441	-0.872	7.067	-5.375	1.00	23.44	O
ATOM	868	N	LEU	A	442	-0.476	9.040	-4.369	1.00	20.94	N
ATOM	869	CA	LEU	A	442	-1.310	8.653	-3.219	1.00	24.86	C
ATOM	870	CB	LEU	A	442	-1.233	9.698	-2.115	1.00	22.54	C
ATOM	871	CG	LEU	A	442	0.100	9.753	-1.362	1.00	22.80	C
ATOM	872	CD1	LEU	A	442	0.125	10.921	-0.355	1.00	22.67	C
ATOM	873	CD2	LEU	A	442	0.315	8.398	-0.661	1.00	23.13	C
ATOM	874	C	LEU	A	442	-2.761	8.469	-3.667	1.00	25.24	C
ATOM	875	O	LEU	A	442	-3.454	7.581	-3.187	1.00	22.68	O
ATOM	876	N	HIS	A	443	-3.228	9.290	-4.605	1.00	23.39	N
ATOM	877	CA	HIS	A	443	-4.607	9.115	-5.069	1.00	22.12	C
ATOM	878	CB	HIS	A	443	-5.024	10.280	-5.985	1.00	27.77	C
ATOM	879	CG	HIS	A	443	-6.388	10.101	-6.573	1.00	28.68	C
ATOM	880	CD2	HIS	A	443	-7.565	9.739	-6.004	1.00	27.01	C
ATOM	881	ND1	HIS	A	443	-6.628	10.196	-7.929	1.00	24.79	N
ATOM	882	CE1	HIS	A	443	-7.893	9.897	-8.171	1.00	24.33	C
ATOM	883	NE2	HIS	A	443	-8.484	9.613	-7.021	1.00	22.99	N
ATOM	884	C	HIS	A	443	-4.781	7.762	-5.781	1.00	22.67	C
ATOM	885	O	HIS	A	443	-5.792	7.077	-5.600	1.00	21.81	O
ATOM	886	N	GLN	A	444	-3.791	7.354	-6.569	1.00	22.84	N
ATOM	887	CA	GLN	A	444	-3.855	6.076	-7.251	1.00	18.98	C
ATOM	888	CB	GLN	A	444	-2.637	5.909	-8.152	1.00	23.77	C
ATOM	889	CG	GLN	A	444	-2.679	6.923	-9.303	1.00	23.82	C
ATOM	890	CD	GLN	A	444	-1.445	6.867	-10.130	1.00	29.64	C
ATOM	891	OE1	GLN	A	444	-0.424	6.344	-9.697	1.00	28.87	O
ATOM	892	NE2	GLN	A	444	-1.521	7.419	-11.342	1.00	28.75	N
ATOM	893	C	GLN	A	444	-3.911	4.958	-6.218	1.00	21.47	C
ATOM	894	O	GLN	A	444	-4.682	4.029	-6.354	1.00	22.83	O
ATOM	895	N	VAL	A	445	-3.114	5.094	-5.162	1.00	21.95	N
ATOM	896	CA	VAL	A	445	-3.162	4.075	-4.119	1.00	19.79	C
ATOM	897	CB	VAL	A	445	-2.131	4.359	-3.001	1.00	21.17	C
ATOM	898	CG1	VAL	A	445	-2.309	3.326	-1.862	1.00	22.83	C
ATOM	899	CG2	VAL	A	445	-0.732	4.274	-3.575	1.00	19.35	C
ATOM	900	C	VAL	A	445	-4.576	4.070	-3.510	1.00	20.72	C
ATOM	901	O	VAL	A	445	-5.107	3.002	-3.225	1.00	21.91	C
ATOM	902	N	SER	A	446	-5.184	5.244	-3.316	1.00	18.98	O
ATOM	903	CA	SER	A	446	-6.543	5.260	-2.734	1.00	19.98	N
ATOM	904	CB	SER	A	446	-6.988	6.704	-2.353	1.00	21.69	C
ATOM	905	OG	SER	A	446	-7.327	7.481	-3.468	1.00	24.84	C
ATOM	906	C	SER	A	446	-7.573	4.627	-3.662	1.00	20.82	O
ATOM	907	O	SER	A	446	-8.553	4.037	-3.187	1.00	21.15	O
ATOM	908	N	MET	A	447	-7.366	4.714	-4.974	1.00	19.01	N
ATOM	909	CA	MET	A	447	-8.294	4.078	-5.909	1.00	22.58	C
ATOM	910	CB	MET	A	447	-8.071	4.588	-7.347	1.00	23.29	C
ATOM	911	CG	MET	A	447	-8.540	6.039	-7.513	1.00	27.40	C
ATOM	912	SD	MET	A	447	-8.500	6.538	-9.288	1.00	29.46	S
ATOM	913	CE	MET	A	447	-6.769	6.928	-9.496	1.00	28.17	C

ATOM	914	C	MET	A	447	-8.133	2.558	-5.838	1.00 25.02	C
ATOM	915	O	MET	A	447	-9.114	1.821	-5.859	1.00 22.91	O
ATOM	916	N	GLY	A	448	-6.903	2.076	-5.729	1.00 20.29	N
ATOM	917	CA	GLY	A	448	-6.712	0.644	-5.625	1.00 22.77	C
ATOM	918	C	GLY	A	448	-7.337	0.135	-4.327	1.00 23.66	C
ATOM	919	O	GLY	A	448	-7.963	-0.934	-4.331	1.00 24.13	O
ATOM	920	N	MET	A	449	-7.192	0.892	-3.236	1.00 22.40	N
ATOM	921	CA	MET	A	449	-7.756	0.450	-1.939	1.00 21.23	C
ATOM	922	CB	MET	A	449	-7.139	1.232	-0.775	1.00 20.57	C
ATOM	923	CG	MET	A	449	-5.611	1.012	-0.550	1.00 19.53	C
ATOM	924	SD	MET	A	449	-5.170	-0.771	-0.382	1.00 25.09	S
ATOM	925	CE	MET	A	449	-6.110	-1.175	1.087	1.00 26.33	C
ATOM	926	C	MET	A	449	-9.282	0.566	-1.888	1.00 22.12	C
ATOM	927	O	MET	A	449	-9.964	-0.236	-1.245	1.00 22.36	O
ATOM	928	N	LYS	A	450	-9.832	1.554	-2.578	1.00 21.36	N
ATOM	929	CA	LYS	A	450	-11.276	1.705	-2.642	1.00 22.17	C
ATOM	930	CB	LYS	A	450	-11.616	2.949	-3.457	1.00 24.95	C
ATOM	931	CG	LYS	A	450	-13.113	3.108	-3.668	1.00 34.59	C
ATOM	932	CD	LYS	A	450	-13.388	4.170	-4.678	1.00 35.54	C
ATOM	933	CE	LYS	A	450	-14.854	4.088	-5.081	1.00 43.28	C
ATOM	934	NZ	LYS	A	450	-15.200	5.226	-5.962	1.00 51.23	N
ATOM	935	C	LYS	A	450	-11.811	0.436	-3.328	1.00 20.54	C
ATOM	936	O	LYS	A	450	-12.829	-0.138	-2.926	1.00 23.77	O
ATOM	937	N	TYR	A	451	-11.093	-0.035	-4.339	1.00 22.16	N
ATOM	938	CA	TYR	A	451	-11.490	-1.254	-5.053	1.00 25.84	C
ATOM	939	CB	TYR	A	451	-10.606	-1.466	-6.295	1.00 30.33	C
ATOM	940	CG	TYR	A	451	-10.851	-2.776	-7.036	1.00 26.97	C
ATOM	941	CD1	TYR	A	451	-11.957	-2.942	-7.887	1.00 32.31	C
ATOM	942	CE1	TYR	A	451	-12.156	-4.161	-8.577	1.00 35.26	C
ATOM	943	CD2	TYR	A	451	-9.975	-3.841	-6.887	1.00 29.55	C
ATOM	944	CE2	TYR	A	451	-10.171	-5.039	-7.538	1.00 38.20	C
ATOM	945	CZ	TYR	A	451	-11.250	-5.202	-8.384	1.00 34.79	C
ATOM	946	OH	TYR	A	451	-11.351	-6.416	-9.028	1.00 33.34	O
ATOM	947	C	TYR	A	451	-11.413	-2.477	-4.156	1.00 25.12	C
ATOM	948	O	TYR	A	451	-12.349	-3.279	-4.111	1.00 21.15	O
ATOM	949	N	LEU	A	452	-10.317	-2.621	-3.411	1.00 23.09	N
ATOM	950	CA	LEU	A	452	-10.190	-3.769	-2.528	1.00 22.43	C
ATOM	951	CB	LEU	A	452	-8.812	-3.775	-1.805	1.00 24.62	C
ATOM	952	CG	LEU	A	452	-7.633	-4.080	-2.723	1.00 29.88	C
ATOM	953	CD1	LEU	A	452	-6.355	-3.885	-1.901	1.00 40.57	C
ATOM	954	CD2	LEU	A	452	-7.706	-5.499	-3.261	1.00 37.63	C
ATOM	955	C	LEU	A	452	-11.289	-3.770	-1.487	1.00 23.29	C
ATOM	956	O	LEU	A	452	-11.835	-4.835	-1.160	1.00 24.20	O
ATOM	957	N	GLU	A	453	-11.615	-2.586	-0.966	1.00 21.59	N
ATOM	958	CA	GLU	A	453	-12.644	-2.465	0.044	1.00 23.71	C
ATOM	959	CB	GLU	A	453	-12.707	-1.020	0.530	1.00 26.43	C
ATOM	960	CG	GLU	A	453	-13.831	-0.730	1.519	1.00 27.65	C
ATOM	961	CD	GLU	A	453	-13.831	0.727	1.990	1.00 34.87	C
ATOM	962	OE1	GLU	A	453	-14.451	1.582	1.298	1.00 33.02	O
ATOM	963	OE2	GLU	A	453	-13.200	1.012	3.042	1.00 30.22	O
ATOM	964	C	GLU	A	453	-14.014	-2.901	-0.520	1.00 27.31	C
ATOM	965	O	GLU	A	453	-14.763	-3.656	0.129	1.00 25.17	O
ATOM	966	N	GLU	A	454	-14.348	-2.407	-1.706	1.00 22.10	N
ATOM	967	CA	GLU	A	454	-15.640	-2.769	-2.310	1.00 25.66	C
ATOM	968	CB	GLU	A	454	-15.871	-1.997	-3.619	1.00 31.24	C
ATOM	969	CG	GLU	A	454	-14.964	-2.392	-4.754	1.00 42.57	C
ATOM	970	CD	GLU	A	454	-15.261	-1.624	-6.046	1.00 58.39	C
ATOM	971	OE1	GLU	A	454	-15.273	-0.363	-6.015	1.00 51.95	O
ATOM	972	OE2	GLU	A	454	-15.472	-2.287	-7.094	1.00 58.17	O
ATOM	973	C	GLU	A	454	-15.721	-4.263	-2.581	1.00 31.04	C
ATOM	974	O	GLU	A	454	-16.810	-4.837	-2.583	1.00 30.48	O
ATOM	975	N	LYS	A	455	-14.583	-4.915	-2.799	1.00 24.65	N
ATOM	976	CA	LYS	A	455	-14.580	-6.358	-3.056	1.00 26.01	C
ATOM	977	CB	LYS	A	455	-13.474	-6.742	-4.058	1.00 26.87	C
ATOM	978	CG	LYS	A	455	-13.600	-6.047	-5.435	1.00 32.48	C
ATOM	979	CD	LYS	A	455	-14.919	-6.413	-6.093	1.00 34.46	C
ATOM	980	CE	LYS	A	455	-15.166	-5.643	-7.397	1.00 39.80	C
ATOM	981	NZ	LYS	A	455	-16.498	-6.028	-7.995	1.00 35.47	N

ATOM	982	C	LYS	A	455	-14.402	-7.158	-1.764	1.00	25.88	C
ATOM	983	O	LYS	A	455	-14.205	-8.367	-1.799	1.00	33.28	O
ATOM	984	N	ASN	A	456	-14.484	-6.474	-0.632	1.00	26.80	N
ATOM	985	CA	ASN	A	456	-14.348	-7.110	0.679	1.00	33.33	C
ATOM	986	CB	ASN	A	456	-15.537	-8.042	0.956	1.00	33.66	C
ATOM	987	CG	ASN	A	456	-16.833	-7.293	1.019	1.00	41.21	C
ATOM	988	OD1	ASN	A	456	-17.005	-6.397	1.847	1.00	38.41	O
ATOM	989	ND2	ASN	A	456	-17.763	-7.640	0.128	1.00	43.69	N
ATOM	990	C	ASN	A	456	-13.048	-7.865	0.932	1.00	32.96	C
ATOM	991	O	ASN	A	456	-13.065	-8.982	1.447	1.00	29.31	O
ATOM	992	N	PHE	A	457	-11.925	-7.265	0.539	1.00	25.61	N
ATOM	993	CA	PHE	A	457	-10.633	-7.871	0.827	1.00	23.17	C
ATOM	994	CB	PHE	A	457	-9.823	-8.104	-0.457	1.00	24.54	C
ATOM	995	CG	PHE	A	457	-10.302	-9.259	-1.274	1.00	27.01	C
ATOM	996	CD1	PHE	A	457	-11.141	-9.064	-2.372	1.00	38.40	C
ATOM	997	CD2	PHE	A	457	-9.912	-10.546	-0.952	1.00	30.92	C
ATOM	998	CE1	PHE	A	457	-11.573	-10.154	-3.131	1.00	40.99	C
ATOM	999	CE2	PHE	A	457	-10.338	-11.633	-1.702	1.00	39.35	C
ATOM	1000	CZ	PHE	A	457	-11.169	-11.435	-2.792	1.00	32.26	C
ATOM	1001	C	PHE	A	457	-9.876	-6.876	1.724	1.00	22.95	C
ATOM	1002	O	PHE	A	457	-10.006	-5.666	1.538	1.00	26.81	O
ATOM	1003	N	VAL	A	458	-9.095	-7.404	2.677	1.00	22.07	N
ATOM	1004	CA	VAL	A	458	-8.271	-6.587	3.574	1.00	18.40	C
ATOM	1005	CB	VAL	A	458	-8.476	-6.999	5.067	1.00	24.28	C
ATOM	1006	CG1	VAL	A	458	-7.490	-6.239	5.978	1.00	19.09	C
ATOM	1007	CG2	VAL	A	458	-9.885	-6.680	5.496	1.00	24.91	C
ATOM	1008	C	VAL	A	458	-6.811	-6.870	3.172	1.00	21.95	C
ATOM	1009	O	VAL	A	458	-6.412	-8.007	3.081	1.00	22.78	O
ATOM	1010	N	HIS	A	459	-6.017	-5.836	2.953	1.00	23.11	N
ATOM	1011	CA	HIS	A	459	-4.620	-6.058	2.514	1.00	22.90	C
ATOM	1012	CB	HIS	A	459	-4.106	-4.777	1.821	1.00	25.33	C
ATOM	1013	CG	HIS	A	459	-2.735	-4.915	1.233	1.00	27.05	C
ATOM	1014	CD2	HIS	A	459	-2.319	-4.984	-0.055	1.00	35.51	C
ATOM	1015	ND1	HIS	A	459	-1.598	-4.995	2.004	1.00	30.45	N
ATOM	1016	CE1	HIS	A	459	-0.539	-5.097	1.218	1.00	30.89	C
ATOM	1017	NE2	HIS	A	459	-0.950	-5.091	-0.037	1.00	27.20	N
ATOM	1018	C	HIS	A	459	-3.726	-6.406	3.702	1.00	22.15	C
ATOM	1019	O	HIS	A	459	-2.926	-7.373	3.669	1.00	26.50	O
ATOM	1020	N	ARG	A	460	-3.870	-5.592	4.743	1.00	22.61	N
ATOM	1021	CA	ARG	A	460	-3.160	-5.697	6.007	1.00	21.98	C
ATOM	1022	CB	ARG	A	460	-3.202	-7.138	6.526	1.00	27.77	C
ATOM	1023	CG	ARG	A	460	-2.704	-7.226	7.957	1.00	39.24	C
ATOM	1024	CD	ARG	A	460	-2.722	-8.632	8.504	1.00	31.08	C
ATOM	1025	NE	ARG	A	460	-1.706	-8.745	9.539	1.00	33.21	N
ATOM	1026	CZ	ARG	A	460	-1.459	-9.857	10.236	1.00	39.79	C
ATOM	1027	NH1	ARG	A	460	-2.161	-10.955	10.014	1.00	32.10	N
ATOM	1028	NH2	ARG	A	460	-0.492	-9.866	11.146	1.00	40.69	N
ATOM	1029	C	ARG	A	460	-1.706	-5.211	6.022	1.00	28.94	C
ATOM	1030	O	ARG	A	460	-1.177	-4.874	7.079	1.00	36.64	O
ATOM	1031	N	ASP	A	461	-1.072	-5.145	4.861	1.00	24.64	N
ATOM	1032	CA	ASP	A	461	0.325	-4.733	4.836	1.00	26.58	C
ATOM	1033	CB	ASP	A	461	1.172	-5.943	4.374	1.00	27.03	C
ATOM	1034	CG	ASP	A	461	2.667	-5.827	4.743	1.00	38.59	C
ATOM	1035	OD1	ASP	A	461	3.050	-4.953	5.551	1.00	48.65	O
ATOM	1036	OD2	ASP	A	461	3.468	-6.646	4.224	1.00	49.76	O
ATOM	1037	C	ASP	A	461	0.521	-3.500	3.932	1.00	27.57	C
ATOM	1038	O	ASP	A	461	1.524	-3.370	3.237	1.00	26.49	O
ATOM	1039	N	LEU	A	462	-0.429	-2.572	3.956	1.00	22.27	N
ATOM	1040	CA	LEU	A	462	-0.278	-1.380	3.139	1.00	21.53	C
ATOM	1041	CB	LEU	A	462	-1.636	-0.666	2.987	1.00	22.43	C
ATOM	1042	CG	LEU	A	462	-1.648	0.602	2.128	1.00	30.85	C
ATOM	1043	CD1	LEU	A	462	-1.215	0.224	0.715	1.00	29.37	C
ATOM	1044	CD2	LEU	A	462	-3.042	1.270	2.133	1.00	27.57	C
ATOM	1045	C	LEU	A	462	0.779	-0.477	3.804	1.00	22.66	C
ATOM	1046	O	LEU	A	462	0.671	-0.125	4.950	1.00	26.45	O
ATOM	1047	N	ALA	A	463	1.832	-0.159	3.063	1.00	21.02	N
ATOM	1048	CA	ALA	A	463	2.926	0.688	3.572	1.00	19.38	C
ATOM	1049	CB	ALA	A	463	3.865	-0.138	4.481	1.00	20.15	C

ATOM	1050	C	ALA	A	463	3.669	1.169	2.323	1.00	17.38	C
ATOM	1051	O	ALA	A	463	3.586	0.534	1.274	1.00	21.49	O
ATOM	1052	N	ALA	A	464	4.383	2.277	2.438	1.00	20.81	N
ATOM	1053	CA	ALA	A	464	5.062	2.797	1.271	1.00	22.24	C
ATOM	1054	CB	ALA	A	464	5.810	4.094	1.651	1.00	19.74	C
ATOM	1055	C	ALA	A	464	6.005	1.777	0.641	1.00	23.62	C
ATOM	1056	O	ALA	A	464	6.180	1.782	-0.571	1.00	22.85	O
ATOM	1057	N	ARG	A	465	6.611	0.915	1.457	1.00	23.55	N
ATOM	1058	CA	ARG	A	465	7.528	-0.112	0.962	1.00	22.78	C
ATOM	1059	CB	ARG	A	465	8.203	-0.852	2.133	1.00	26.22	C
ATOM	1060	CG	ARG	A	465	7.254	-1.662	3.026	1.00	22.40	C
ATOM	1061	CD	ARG	A	465	7.980	-2.238	4.272	1.00	27.73	C
ATOM	1062	NE	ARG	A	465	7.030	-2.873	5.180	1.00	32.59	N
ATOM	1063	CZ	ARG	A	465	6.337	-2.232	6.126	1.00	41.47	C
ATOM	1064	NH1	ARG	A	465	6.491	-0.928	6.320	1.00	34.18	N
ATOM	1065	NH2	ARG	A	465	5.441	-2.887	6.841	1.00	40.07	N
ATOM	1066	C	ARG	A	465	6.814	-1.136	0.084	1.00	24.95	C
ATOM	1067	O	ARG	A	465	7.461	-1.867	-0.673	1.00	25.58	O
ATOM	1068	N	ASN	A	466	5.484	-1.203	0.199	1.00	24.98	N
ATOM	1069	CA	ASN	A	466	4.715	-2.149	-0.603	1.00	23.15	C
ATOM	1070	CB	ASN	A	466	3.785	-2.982	0.276	1.00	20.54	C
ATOM	1071	CG	ASN	A	466	4.537	-3.987	1.118	1.00	29.73	C
ATOM	1072	OD1	ASN	A	466	5.600	-4.469	0.710	1.00	26.55	O
ATOM	1073	ND2	ASN	A	466	4.000	-4.310	2.302	1.00	25.54	N
ATOM	1074	C	ASN	A	466	3.947	-1.509	-1.752	1.00	23.75	C
ATOM	1075	O	ASN	A	466	3.185	-2.171	-2.442	1.00	24.79	O
ATOM	1076	N	VAL	A	467	4.170	-0.220	-1.959	1.00	21.31	N
ATOM	1077	CA	VAL	A	467	3.561	0.462	-3.086	1.00	19.34	C
ATOM	1078	CB	VAL	A	467	3.127	1.872	-2.699	1.00	21.47	C
ATOM	1079	CG1	VAL	A	467	2.736	2.647	-3.979	1.00	22.29	C
ATOM	1080	CG2	VAL	A	467	1.957	1.792	-1.696	1.00	19.95	C
ATOM	1081	C	VAL	A	467	4.733	0.538	-4.076	1.00	22.01	C
ATOM	1082	O	VAL	A	467	5.817	1.025	-3.721	1.00	22.82	O
ATOM	1083	N	LEU	A	468	4.524	0.036	-5.290	1.00	21.63	N
ATOM	1084	CA	LEU	A	468	5.601	0.021	-6.286	1.00	25.97	C
ATOM	1085	CB	LEU	A	468	5.828	-1.399	-6.801	1.00	21.35	C
ATOM	1086	CG	LEU	A	468	6.073	-2.498	-5.767	1.00	25.31	C
ATOM	1087	CD1	LEU	A	468	5.995	-3.859	-6.430	1.00	25.16	C
ATOM	1088	CD2	LEU	A	468	7.434	-2.267	-5.110	1.00	27.20	C
ATOM	1089	C	LEU	A	468	5.285	0.920	-7.465	1.00	29.27	C
ATOM	1090	O	LEU	A	468	4.143	1.006	-7.884	1.00	26.29	O
ATOM	1091	N	LEU	A	469	6.311	1.554	-8.035	1.00	24.41	N
ATOM	1092	CA	LEU	A	469	6.063	2.440	-9.156	1.00	25.24	C
ATOM	1093	CB	LEU	A	469	6.886	3.714	-8.973	1.00	28.20	C
ATOM	1094	CG	LEU	A	469	6.583	4.441	-7.661	1.00	40.39	C
ATOM	1095	CD1	LEU	A	469	7.566	5.547	-7.471	1.00	42.75	C
ATOM	1096	CD2	LEU	A	469	5.180	5.007	-7.681	1.00	36.92	C
ATOM	1097	C	LEU	A	469	6.356	1.844	-10.518	1.00	25.99	C
ATOM	1098	O	LEU	A	469	7.411	1.237	-10.729	1.00	27.91	O
ATOM	1099	N	VAL	A	470	5.416	1.985	-11.445	1.00	27.37	N
ATOM	1100	CA	VAL	A	470	5.662	1.526	-12.795	1.00	27.70	C
ATOM	1101	CB	VAL	A	470	4.369	1.352	-13.589	1.00	30.57	C
ATOM	1102	CG1	VAL	A	470	4.693	1.012	-15.042	1.00	35.99	C
ATOM	1103	CG2	VAL	A	470	3.536	0.219	-12.963	1.00	28.74	C
ATOM	1104	C	VAL	A	470	6.517	2.663	-13.384	1.00	32.73	C
ATOM	1105	O	VAL	A	470	7.467	2.415	-14.137	1.00	35.56	O
ATOM	1106	N	ASN	A	471	6.172	3.895	-13.012	1.00	30.05	N
ATOM	1107	CA	ASN	A	471	6.889	5.122	-13.415	1.00	35.49	C
ATOM	1108	CB	ASN	A	471	6.441	5.610	-14.805	1.00	38.79	C
ATOM	1109	CG	ASN	A	471	4.941	5.766	-14.912	1.00	38.59	C
ATOM	1110	OD1	ASN	A	471	4.246	4.841	-15.320	1.00	61.19	O
ATOM	1111	ND2	ASN	A	471	4.432	6.917	-14.518	1.00	37.18	N
ATOM	1112	C	ASN	A	471	6.561	6.186	-12.366	1.00	34.10	C
ATOM	1113	O	ASN	A	471	5.766	5.925	-11.458	1.00	31.54	O
ATOM	1114	N	ARG	A	472	7.144	7.383	-12.468	1.00	31.44	N
ATOM	1115	CA	ARG	A	472	6.889	8.423	-11.467	1.00	34.23	C
ATOM	1116	CB	ARG	A	472	7.812	9.628	-11.699	1.00	36.29	C
ATOM	1117	CG	ARG	A	472	7.539	10.352	-13.002	1.00	38.64	C

ATOM	1118	CD	ARG	A	472	8.440	11.577	-13.126	1.00	42.01	C
ATOM	1119	NE	ARG	A	472	7.960	12.686	-12.310	1.00	42.62	N
ATOM	1120	CZ	ARG	A	472	8.611	13.835	-12.142	1.00	49.56	C
ATOM	1121	NH1	ARG	A	472	9.789	14.036	-12.734	1.00	41.21	N
ATOM	1122	NH2	ARG	A	472	8.082	14.791	-11.395	1.00	45.67	N
ATOM	1123	C	ARG	A	472	5.442	8.907	-11.393	1.00	23.39	C
ATOM	1124	O	ARG	A	472	5.087	9.644	-10.491	1.00	29.27	O
ATOM	1125	N	HIS	A	473	4.621	8.504	-12.357	1.00	26.03	N
ATOM	1126	CA	HIS	A	473	3.234	8.911	-12.392	1.00	32.63	C
ATOM	1127	CB	HIS	A	473	2.947	9.729	-13.680	1.00	27.76	C
ATOM	1128	CG	HIS	A	473	3.693	11.026	-13.743	1.00	31.49	C
ATOM	1129	CD2	HIS	A	473	4.728	11.426	-14.522	1.00	40.44	C
ATOM	1130	ND1	HIS	A	473	3.462	12.056	-12.858	1.00	33.49	N
ATOM	1131	CE1	HIS	A	473	4.327	13.031	-13.082	1.00	42.59	C
ATOM	1132	NE2	HIS	A	473	5.108	12.673	-14.086	1.00	41.30	N
ATOM	1133	C	HIS	A	473	2.296	7.710	-12.329	1.00	28.13	C
ATOM	1134	O	HIS	A	473	1.105	7.842	-12.651	1.00	25.55	O
ATOM	1135	N	TYR	A	474	2.813	6.547	-11.928	1.00	26.97	N
ATOM	1136	CA	TYR	A	474	1.957	5.357	-11.889	1.00	29.51	C
ATOM	1137	CB	TYR	A	474	1.991	4.652	-13.250	1.00	26.22	C
ATOM	1138	CG	TYR	A	474	0.982	3.515	-13.472	1.00	30.97	C
ATOM	1139	CD1	TYR	A	474	-0.077	3.274	-12.582	1.00	28.77	C
ATOM	1140	CE1	TYR	A	474	-1.001	2.218	-12.823	1.00	31.08	C
ATOM	1141	CD2	TYR	A	474	1.091	2.689	-14.596	1.00	33.81	C
ATOM	1142	CE2	TYR	A	474	0.191	1.658	-14.838	1.00	34.98	C
ATOM	1143	CZ	TYR	A	474	-0.853	1.418	-13.960	1.00	33.21	C
ATOM	1144	OH	TYR	A	474	-1.723	0.375	-14.256	1.00	31.45	O
ATOM	1145	C	TYR	A	474	2.358	4.376	-10.789	1.00	25.47	C
ATOM	1146	O	TYR	A	474	3.336	3.636	-10.932	1.00	28.97	O
ATOM	1147	N	ALA	A	475	1.571	4.374	-9.710	1.00	22.78	N
ATOM	1148	CA	ALA	A	475	1.837	3.495	-8.577	1.00	26.62	C
ATOM	1149	CB	ALA	A	475	1.696	4.297	-7.265	1.00	27.18	C
ATOM	1150	C	ALA	A	475	0.897	2.280	-8.553	1.00	28.20	C
ATOM	1151	O	ALA	A	475	-0.234	2.341	-9.045	1.00	25.92	O
ATOM	1152	N	LYS	A	476	1.380	1.169	-7.990	1.00	24.41	N
ATOM	1153	CA	LYS	A	476	0.569	-0.039	-7.855	1.00	23.63	C
ATOM	1154	CB	LYS	A	476	0.957	-1.092	-8.912	1.00	26.51	C
ATOM	1155	CG	LYS	A	476	0.418	-0.795	-10.305	1.00	27.53	C
ATOM	1156	CD	LYS	A	476	0.985	-1.811	-11.310	1.00	32.34	C
ATOM	1157	CE	LYS	A	476	0.273	-1.748	-12.657	1.00	36.56	C
ATOM	1158	NZ	LYS	A	476	-0.989	-2.542	-12.605	1.00	37.90	N
ATOM	1159	C	LYS	A	476	0.772	-0.657	-6.477	1.00	25.52	C
ATOM	1160	O	LYS	A	476	1.898	-0.684	-5.956	1.00	25.22	O
ATOM	1161	N	ILE	A	477	-0.309	-1.172	-5.896	1.00	22.11	N
ATOM	1162	CA	ILE	A	477	-0.214	-1.800	-4.580	1.00	24.01	C
ATOM	1163	CB	ILE	A	477	-1.577	-1.846	-3.915	1.00	21.78	C
ATOM	1164	CG2	ILE	A	477	-1.499	-2.642	-2.596	1.00	25.26	C
ATOM	1165	CG1	ILE	A	477	-2.081	-0.417	-3.708	1.00	20.73	C
ATOM	1166	CD1	ILE	A	477	-3.578	-0.332	-3.534	1.00	22.58	C
ATOM	1167	C	ILE	A	477	0.267	-3.223	-4.766	1.00	24.46	C
ATOM	1168	O	ILE	A	477	-0.216	-3.919	-5.654	1.00	22.86	O
ATOM	1169	N	SER	A	478	1.214	-3.666	-3.932	1.00	22.32	N
ATOM	1170	CA	SER	A	478	1.691	-5.039	-4.071	1.00	22.20	C
ATOM	1171	CB	SER	A	478	3.097	-5.049	-4.649	1.00	28.05	C
ATOM	1172	OG	SER	A	478	3.965	-4.509	-3.674	1.00	38.71	O
ATOM	1173	C	SER	A	478	1.723	-5.787	-2.738	1.00	26.29	C
ATOM	1174	O	SER	A	478	1.311	-5.261	-1.697	1.00	25.87	O
ATOM	1175	N	ASP	A	479	2.247	-7.010	-2.810	1.00	23.81	N
ATOM	1176	CA	ASP	A	479	2.394	-7.959	-1.690	1.00	25.45	C
ATOM	1177	CB	ASP	A	479	3.465	-7.519	-0.666	1.00	24.64	C
ATOM	1178	CG	ASP	A	479	3.850	-8.676	0.288	1.00	35.61	C
ATOM	1179	OD1	ASP	A	479	3.141	-9.710	0.289	1.00	30.47	O
ATOM	1180	OD2	ASP	A	479	4.860	-8.567	1.018	1.00	31.61	O
ATOM	1181	C	ASP	A	479	1.099	-8.294	-0.952	1.00	21.75	C
ATOM	1182	O	ASP	A	479	0.819	-7.751	0.144	1.00	21.47	O
ATOM	1183	N	PHE	A	480	0.359	-9.246	-1.524	1.00	24.40	N
ATOM	1184	CA	PHE	A	480	-0.905	-9.719	-0.946	1.00	27.55	C
ATOM	1185	CB	PHE	A	480	-1.910	-9.973	-2.077	1.00	22.84	C

ATOM	1186	CG	PHE	A	480	-2.335	-8.709	-2.776	1.00	25.54	C
ATOM	1187	CD1	PHE	A	480	-3.472	-7.999	-2.373	1.00	37.22	C
ATOM	1188	CD2	PHE	A	480	-1.531	-8.165	-3.774	1.00	29.75	C
ATOM	1189	CE1	PHE	A	480	-3.788	-6.767	-2.950	1.00	36.53	C
ATOM	1190	CE2	PHE	A	480	-1.841	-6.925	-4.351	1.00	31.15	C
ATOM	1191	CZ	PHE	A	480	-2.956	-6.229	-3.945	1.00	30.92	C
ATOM	1192	C	PHE	A	480	-0.734	-10.978	-0.070	1.00	22.25	C
ATOM	1193	O	PHE	A	480	-1.693	-11.697	0.201	1.00	28.80	O
ATOM	1194	N	GLY	A	481	0.494	-11.200	0.395	1.00	26.68	N
ATOM	1195	CA	GLY	A	481	0.808	-12.354	1.234	1.00	25.28	C
ATOM	1196	C	GLY	A	481	0.041	-12.422	2.553	1.00	29.85	C
ATOM	1197	O	GLY	A	481	-0.094	-13.489	3.125	1.00	28.84	O
ATOM	1198	N	LEU	A	482	-0.455	-11.293	3.049	1.00	21.56	N
ATOM	1199	CA	LEU	A	482	-1.217	-11.299	4.316	1.00	23.95	C
ATOM	1200	CB	LEU	A	482	-0.608	-10.287	5.304	1.00	25.94	C
ATOM	1201	CG	LEU	A	482	0.789	-10.660	5.792	1.00	31.12	C
ATOM	1202	CD1	LEU	A	482	1.418	-9.482	6.554	1.00	34.67	C
ATOM	1203	CD2	LEU	A	482	0.680	-11.884	6.675	1.00	35.08	C
ATOM	1204	C	LEU	A	482	-2.667	-10.925	4.097	1.00	21.10	C
ATOM	1205	O	LEU	A	482	-3.441	-10.766	5.050	1.00	26.73	O
ATOM	1206	N	SER	A	483	-3.050	-10.794	2.837	1.00	21.83	N
ATOM	1207	CA	SER	A	483	-4.409	-10.375	2.518	1.00	17.76	C
ATOM	1208	CB	SER	A	483	-4.465	-9.958	1.042	1.00	22.28	C
ATOM	1209	OG	SER	A	483	-3.595	-8.851	0.860	1.00	29.25	O
ATOM	1210	C	SER	A	483	-5.440	-11.475	2.785	1.00	21.06	C
ATOM	1211	O	SER	A	483	-5.128	-12.645	2.739	1.00	24.20	O
ATOM	1212	N	LYS	A	484	-6.681	-11.071	3.034	1.00	20.71	N
ATOM	1213	CA	LYS	A	484	-7.738	-12.041	3.291	1.00	21.00	C
ATOM	1214	CB	LYS	A	484	-7.862	-12.318	4.791	1.00	24.78	C
ATOM	1215	CG	LYS	A	484	-6.650	-13.105	5.362	1.00	38.83	C
ATOM	1216	CD	LYS	A	484	-6.770	-13.393	6.859	1.00	45.27	C
ATOM	1217	CE	LYS	A	484	-5.677	-14.378	7.302	1.00	43.33	C
ATOM	1218	NZ	LYS	A	484	-4.326	-14.049	6.778	1.00	56.25	N
ATOM	1219	C	LYS	A	484	-9.076	-11.545	2.768	1.00	25.54	C
ATOM	1220	O	LYS	A	484	-9.320	-10.348	2.677	1.00	26.31	O
ATOM	1221	N	ALA	A	485	-9.941	-12.491	2.434	1.00	23.65	N
ATOM	1222	CA	ALA	A	485	-11.280	-12.138	1.974	1.00	22.67	C
ATOM	1223	CB	ALA	A	485	-11.814	-13.210	0.995	1.00	31.69	C
ATOM	1224	C	ALA	A	485	-12.144	-12.086	3.249	1.00	31.19	C
ATOM	1225	O	ALA	A	485	-12.006	-12.931	4.136	1.00	29.37	O
ATOM	1226	N	LEU	A	486	-12.995	-11.073	3.349	1.00	23.82	N
ATOM	1227	CA	LEU	A	486	-13.873	-10.926	4.518	1.00	20.69	C
ATOM	1228	CB	LEU	A	486	-14.113	-9.435	4.825	1.00	28.46	C
ATOM	1229	CG	LEU	A	486	-13.031	-8.604	5.532	1.00	31.01	C
ATOM	1230	CD1	LEU	A	486	-13.418	-7.137	5.591	1.00	36.09	C
ATOM	1231	CD2	LEU	A	486	-12.840	-9.129	6.923	1.00	37.43	C
ATOM	1232	C	LEU	A	486	-15.239	-11.583	4.288	1.00	31.06	C
ATOM	1233	O	LEU	A	486	-15.911	-11.953	5.235	1.00	33.37	O
ATOM	1234	N	GLY	A	487	-15.651	-11.715	3.031	1.00	28.59	N
ATOM	1235	CA	GLY	A	487	-16.955	-12.284	2.753	1.00	33.58	C
ATOM	1236	C	GLY	A	487	-18.031	-11.345	3.283	1.00	38.11	C
ATOM	1237	O	GLY	A	487	-17.980	-10.144	3.077	1.00	36.30	O
ATOM	1238	N	ALA	A	488	-18.987	-11.910	4.004	1.00	38.66	N
ATOM	1239	CA	ALA	A	488	-20.092	-11.130	4.556	1.00	40.22	C
ATOM	1240	CB	ALA	A	488	-21.287	-12.045	4.812	1.00	46.29	C
ATOM	1241	C	ALA	A	488	-19.733	-10.388	5.843	1.00	40.58	C
ATOM	1242	O	ALA	A	488	-20.483	-9.532	6.295	1.00	40.10	O
ATOM	1243	N	ASP	A	489	-18.578	-10.699	6.422	1.00	36.35	N
ATOM	1244	CA	ASP	A	489	-18.160	-10.041	7.672	1.00	35.41	C
ATOM	1245	CB	ASP	A	489	-17.192	-10.955	8.431	1.00	37.29	C
ATOM	1246	CG	ASP	A	489	-17.782	-12.314	8.686	1.00	49.00	C
ATOM	1247	OD1	ASP	A	489	-19.013	-12.383	8.909	1.00	49.08	O
ATOM	1248	OD2	ASP	A	489	-17.018	-13.305	8.680	1.00	50.85	O
ATOM	1249	C	ASP	A	489	-17.508	-8.676	7.484	1.00	30.55	C
ATOM	1250	O	ASP	A	489	-16.974	-8.388	6.427	1.00	32.36	O
ATOM	1251	N	ASP	A	490	-17.538	-7.845	8.529	1.00	28.02	N
ATOM	1252	CA	ASP	A	490	-16.923	-6.527	8.441	1.00	31.41	C
ATOM	1253	CB	ASP	A	490	-17.768	-5.486	9.178	1.00	38.68	C

ATOM	1254	CG	ASP	A	490	-17.934	-5.812	10.630	1.00	48.46	C
ATOM	1255	OD1	ASP	A	490	-18.996	-5.471	11.213	1.00	57.52	O
ATOM	1256	OD2	ASP	A	490	-16.999	-6.397	11.198	1.00	54.69	O
ATOM	1257	C	ASP	A	490	-15.492	-6.523	8.983	1.00	26.85	C
ATOM	1258	O	ASP	A	490	-14.799	-5.512	8.906	1.00	24.78	O
ATOM	1259	N	SER	A	491	-15.046	-7.652	9.521	1.00	23.91	N
ATOM	1260	CA	SER	A	491	-13.666	-7.760	10.031	1.00	22.38	C
ATOM	1261	CB	SER	A	491	-13.522	-6.993	11.336	1.00	29.00	C
ATOM	1262	OG	SER	A	491	-14.280	-7.634	12.371	1.00	32.97	O
ATOM	1263	C	SER	A	491	-13.333	-9.202	10.309	1.00	29.41	C
ATOM	1264	O	SER	A	491	-14.204	-10.076	10.200	1.00	25.81	O
ATOM	1265	N	TYR	A	492	-12.068	-9.462	10.640	1.00	23.00	N
ATOM	1266	CA	TYR	A	492	-11.679	-10.788	11.033	1.00	26.00	C
ATOM	1267	CB	TYR	A	492	-11.165	-11.647	9.858	1.00	26.94	C
ATOM	1268	CG	TYR	A	492	-9.811	-11.265	9.328	1.00	26.14	C
ATOM	1269	CD1	TYR	A	492	-8.639	-11.830	9.855	1.00	24.16	C
ATOM	1270	CE1	TYR	A	492	-7.378	-11.414	9.419	1.00	28.54	C
ATOM	1271	CD2	TYR	A	492	-9.693	-10.285	8.348	1.00	25.38	C
ATOM	1272	CE2	TYR	A	492	-8.424	-9.859	7.902	1.00	23.56	C
ATOM	1273	CZ	TYR	A	492	-7.282	-10.428	8.447	1.00	26.57	C
ATOM	1274	OH	TYR	A	492	-6.040	-9.993	8.045	1.00	24.90	O
ATOM	1275	C	TYR	A	492	-10.630	-10.613	12.122	1.00	23.17	C
ATOM	1276	O	TYR	A	492	-10.082	-9.521	12.308	1.00	22.18	O
ATOM	1277	N	TYR	A	493	-10.404	-11.690	12.865	1.00	21.40	N
ATOM	1278	CA	TYR	A	493	-9.406	-11.705	13.943	1.00	18.61	C
ATOM	1279	CB	TYR	A	493	-10.015	-12.168	15.262	1.00	23.77	C
ATOM	1280	CG	TYR	A	493	-10.965	-11.174	15.837	1.00	24.82	C
ATOM	1281	CD1	TYR	A	493	-12.229	-11.002	15.282	1.00	26.28	C
ATOM	1282	CE1	TYR	A	493	-13.105	-10.061	15.789	1.00	33.92	C
ATOM	1283	CD2	TYR	A	493	-10.598	-10.375	16.921	1.00	24.00	C
ATOM	1284	CE2	TYR	A	493	-11.468	-9.431	17.439	1.00	29.62	C
ATOM	1285	CZ	TYR	A	493	-12.719	-9.284	16.868	1.00	33.02	C
ATOM	1286	OH	TYR	A	493	-13.592	-8.384	17.410	1.00	32.06	O
ATOM	1287	C	TYR	A	493	-8.394	-12.708	13.459	1.00	19.01	C
ATOM	1288	O	TYR	A	493	-8.749	-13.842	13.091	1.00	22.83	O
ATOM	1289	N	THR	A	494	-7.141	-12.272	13.400	1.00	26.38	N
ATOM	1290	CA	THR	A	494	-6.077	-13.079	12.834	1.00	32.64	C
ATOM	1291	CB	THR	A	494	-5.029	-12.172	12.119	1.00	31.23	C
ATOM	1292	OG1	THR	A	494	-4.099	-12.987	11.401	1.00	41.68	O
ATOM	1293	CG2	THR	A	494	-4.270	-11.355	13.123	1.00	33.57	C
ATOM	1294	C	THR	A	494	-5.332	-13.934	13.830	1.00	34.49	C
ATOM	1295	O	THR	A	494	-5.210	-13.605	15.005	1.00	28.24	O
ATOM	1296	N	ALA	A	495	-4.747	-15.006	13.322	1.00	44.02	N
ATOM	1297	CA	ALA	A	495	-3.959	-15.870	14.166	1.00	49.59	C
ATOM	1298	CB	ALA	A	495	-3.887	-17.248	13.552	1.00	46.73	C
ATOM	1299	C	ALA	A	495	-2.562	-15.276	14.307	1.00	50.58	C
ATOM	1300	O	ALA	A	495	-2.108	-14.536	13.439	1.00	49.05	O
ATOM	1301	N	ARG	A	496	-1.899	-15.593	15.409	1.00	54.28	N
ATOM	1302	CA	ARG	A	496	-0.552	-15.110	15.668	1.00	58.65	C
ATOM	1303	CB	ARG	A	496	-0.261	-15.109	17.173	1.00	60.21	C
ATOM	1304	CG	ARG	A	496	0.432	-13.854	17.698	1.00	65.46	C
ATOM	1305	CD	ARG	A	496	1.644	-13.487	16.885	1.00	66.41	C
ATOM	1306	NE	ARG,	A	496	2.227	-12.233	17.353	1.00	67.01	N
ATOM	1307	CZ	ARG	A	496	3.254	-11.624	16.771	1.00	70.08	C
ATOM	1308	NH1	ARG	A	496	3.816	-12.156	15.690	1.00	71.57	N
ATOM	1309	NH2	ARG	A	496	3.722	-10.486	17.268	1.00	67.36	N
ATOM	1310	C	ARG	A	496	0.441	-16.048	14.971	1.00	60.54	C
ATOM	1311	O	ARG	A	496	0.365	-17.270	15.112	1.00	59.09	O
ATOM	1312	N	SER	A	497	1.362	-15.475	14.209	1.00	58.17	N
ATOM	1313	CA	SER	A	497	2.370	-16.275	13.523	1.00	60.35	C
ATOM	1314	CB	SER	A	497	2.276	-16.074	12.010	1.00	60.39	C
ATOM	1315	OG	SER	A	497	2.664	-14.760	11.653	1.00	64.92	O
ATOM	1316	C	SER	A	497	3.736	-15.821	14.016	1.00	60.92	C
ATOM	1317	O	SER	A	497	3.836	-14.890	14.817	1.00	58.88	O
ATOM	1318	N	ALA	A	498	4.781	-16.480	13.531	1.00	63.41	N
ATOM	1319	CA	ALA	A	498	6.146	-16.143	13.911	1.00	61.88	C
ATOM	1320	CB	ALA	A	498	7.102	-17.263	13.482	1.00	59.84	C
ATOM	1321	C	ALA	A	498	6.556	-14.827	13.254	1.00	60.58	C

ATOM	1322	O	ALA	A	498	6.132	-14.515	12.138	1.00	60.40	O
ATOM	1323	N	GLY	A	499	7.381	-14.057	13.950	1.00	60.46	N
ATOM	1324	CA	GLY	A	499	7.833	-12.798	13.393	1.00	63.38	C
ATOM	1325	C	GLY	A	499	7.226	-11.608	14.100	1.00	61.34	C
ATOM	1326	O	GLY	A	499	6.240	-11.741	14.827	1.00	64.30	O
ATOM	1327	N	LYS	A	500	7.817	-10.440	13.886	1.00	60.00	N
ATOM	1328	CA	LYS	A	500	7.338	-9.216	14.511	1.00	56.90	C
ATOM	1329	CB	LYS	A	500	8.502	-8.246	14.717	1.00	60.17	C
ATOM	1330	CG	LYS	A	500	9.535	-8.705	15.729	1.00	63.00	C
ATOM	1331	CD	LYS	A	500	8.991	-8.599	17.148	1.00	67.02	C
ATOM	1332	CE	LYS	A	500	10.049	-8.992	18.174	1.00	65.56	C
ATOM	1333	NZ	LYS	A	500	9.537	-8.897	19.573	1.00	68.82	N
ATOM	1334	C	LYS	A	500	6.272	-8.539	13.654	1.00	51.76	C
ATOM	1335	O	LYS	A	500	6.271	-8.656	12.434	1.00	48.14	O
ATOM	1336	N	TRP	A	501	5.363	-7.829	14.311	1.00	47.51	N
ATOM	1337	CA	TRP	A	501	4.307	-7.104	13.602	1.00	46.32	C
ATOM	1338	CB	TRP	A	501	3.028	-7.109	14.441	1.00	41.88	C
ATOM	1339	CG	TRP	A	501	2.225	-8.356	14.335	1.00	37.72	C
ATOM	1340	CD2	TRP	A	501	0.855	-8.518	14.721	1.00	36.73	C
ATOM	1341	CE2	TRP	A	501	0.471	-9.832	14.363	1.00	39.69	C
ATOM	1342	CE3	TRP	A	501	-0.089	-7.679	15.334	1.00	38.48	C
ATOM	1343	CD1	TRP	A	501	2.613	-9.547	13.789	1.00	42.00	C
ATOM	1344	NE1	TRP	A	501	1.562	-10.441	13.797	1.00	38.68	N
ATOM	1345	CZ2	TRP	A	501	-0.821	-10.325	14.593	1.00	35.30	C
ATOM	1346	CZ3	TRP	A	501	-1.379	-8.176	15.565	1.00	32.86	C
ATOM	1347	CH2	TRP	A	501	-1.726	-9.483	15.192	1.00	35.05	C
ATOM	1348	C	TRP	A	501	4.765	-5.658	13.385	1.00	39.20	C
ATOM	1349	O	TRP	A	501	5.361	-5.063	14.279	1.00	42.54	O
ATOM	1350	N	PRO	A	502	4.500	-5.079	12.197	1.00	36.57	N
ATOM	1351	CD	PRO	A	502	3.828	-5.725	11.050	1.00	35.66	C
ATOM	1352	CA	PRO	A	502	4.885	-3.689	11.876	1.00	38.88	C
ATOM	1353	CB	PRO	A	502	4.721	-3.623	10.359	1.00	37.46	C
ATOM	1354	CG	PRO	A	502	3.547	-4.559	10.117	1.00	42.86	C
ATOM	1355	C	PRO	A	502	3.908	-2.772	12.604	1.00	36.51	C
ATOM	1356	O	PRO	A	502	3.018	-2.152	11.988	1.00	28.01	O
ATOM	1357	N	LEU	A	503	4.079	-2.706	13.921	1.00	29.24	N
ATOM	1358	CA	LEU	A	503	3.185	-1.931	14.780	1.00	29.71	C
ATOM	1359	CB	LEU	A	503	3.701	-1.950	16.227	1.00	36.06	C
ATOM	1360	CG	LEU	A	503	3.999	-3.328	16.817	1.00	39.54	C
ATOM	1361	CD1	LEU	A	503	4.596	-3.172	18.215	1.00	48.04	C
ATOM	1362	CD2	LEU	A	503	2.727	-4.145	16.872	1.00	43.63	C
ATOM	1363	C	LEU	A	503	2.962	-0.489	14.364	1.00	25.89	C
ATOM	1364	O	LEU	A	503	1.875	0.057	14.580	1.00	24.95	O
ATOM	1365	N	LYS	A	504	3.979	0.132	13.766	1.00	24.94	N
ATOM	1366	CA	LYS	A	504	3.860	1.527	13.379	1.00	25.26	C
ATOM	1367	CB	LYS	A	504	5.223	2.090	12.978	1.00	28.02	C
ATOM	1368	CG	LYS	A	504	6.170	2.228	14.194	1.00	31.43	C
ATOM	1369	CD	LYS	A	504	7.500	2.881	13.813	1.00	31.17	C
ATOM	1370	CE	LYS	A	504	8.447	2.979	15.011	1.00	36.32	C
ATOM	1371	NZ	LYS	A	504	9.635	3.805	14.649	1.00	38.54	N
ATOM	1372	C	LYS	A	504	2.846	1.772	12.264	1.00	26.30	C
ATOM	1373	O	LYS	A	504	2.453	2.892	12.040	1.00	22.29	O
ATOM	1374	N	TRP	A	505	2.430	0.719	11.581	1.00	22.68	N
ATOM	1375	CA	TRP	A	505	1.437	0.866	10.515	1.00	18.95	C
ATOM	1376	CB	TRP	A	505	1.890	0.096	9.275	1.00	25.33	C
ATOM	1377	CG	TRP	A	505	2.892	0.834	8.461	1.00	25.92	C
ATOM	1378	CD2	TRP	A	505	4.295	0.938	8.717	1.00	24.46	C
ATOM	1379	CE2	TRP	A	505	4.834	1.808	7.739	1.00	23.54	C
ATOM	1380	CE3	TRP	A	505	5.155	0.383	9.681	1.00	26.35	C
ATOM	1381	CD1	TRP	A	505	2.633	1.615	7.365	1.00	19.83	C
ATOM	1382	NE1	TRP	A	505	3.801	2.208	6.926	1.00	24.61	N
ATOM	1383	CZ2	TRP	A	505	6.198	2.138	7.692	1.00	27.89	C
ATOM	1384	CZ3	TRP	A	505	6.516	0.709	9.635	1.00	27.25	C
ATOM	1385	CH2	TRP	A	505	7.024	1.581	8.642	1.00	26.23	C
ATOM	1386	C	TRP	A	505	0.070	0.305	10.971	1.00	22.11	C
ATOM	1387	O	TRP	A	505	-0.926	0.429	10.258	1.00	22.39	O
ATOM	1388	N	TYR	A	506	0.027	-0.266	12.167	1.00	21.52	N
ATOM	1389	CA	TYR	A	506	-1.231	-0.889	12.650	1.00	22.86	C

ATOM	1390	CB	TYR	A	506	-0.859	-2.165	13.442	1.00	21.24	C
ATOM	1391	CG	TYR	A	506	-0.540	-3.393	12.593	1.00	23.75	C
ATOM	1392	CD1	TYR	A	506	-0.335	-3.297	11.221	1.00	25.21	C
ATOM	1393	CE1	TYR	A	506	-0.008	-4.434	10.444	1.00	33.36	C
ATOM	1394	CD2	TYR	A	506	-0.424	-4.659	13.184	1.00	30.33	C
ATOM	1395	CE2	TYR	A	506	-0.113	-5.795	12.413	1.00	33.98	C
ATOM	1396	CZ	TYR	A	506	0.100	-5.674	11.053	1.00	34.14	C
ATOM	1397	OH	TYR	A	506	0.459	-6.784	10.310	1.00	36.03	O
ATOM	1398	C	TYR	A	506	-2.184	-0.017	13.500	1.00	25.61	C
ATOM	1399	O	TYR	A	506	-1.737	0.682	14.412	1.00	24.59	O
ATOM	1400	N	ALA	A	507	-3.490	-0.076	13.209	1.00	21.31	N
ATOM	1401	CA	ALA	A	507	-4.511	0.664	13.950	1.00	21.80	C
ATOM	1402	CB	ALA	A	507	-5.894	0.502	13.254	1.00	18.75	C
ATOM	1403	C	ALA	A	507	-4.570	0.070	15.374	1.00	26.17	C
ATOM	1404	O	ALA	A	507	-4.161	-1.064	15.607	1.00	22.46	O
ATOM	1405	N	PRO	A	508	-5.107	0.831	16.332	1.00	22.10	N
ATOM	1406	CD	PRO	A	508	-5.596	2.214	16.186	1.00	22.87	C
ATOM	1407	CA	PRO	A	508	-5.213	0.370	17.722	1.00	24.97	C
ATOM	1408	CB	PRO	A	508	-5.979	1.499	18.403	1.00	25.74	C
ATOM	1409	CG	PRO	A	508	-5.555	2.711	17.600	1.00	34.90	C
ATOM	1410	C	PRO	A	508	-5.898	-0.978	17.922	1.00	28.04	C
ATOM	1411	O	PRO	A	508	-5.397	-1.819	18.682	1.00	24.23	O
ATOM	1412	N	GLU	A	509	-7.019	-1.193	17.229	1.00	24.59	N
ATOM	1413	CA	GLU	A	509	-7.754	-2.445	17.352	1.00	27.89	C
ATOM	1414	CB	GLU	A	509	-9.128	-2.368	16.654	1.00	27.01	C
ATOM	1415	CG	GLU	A	509	-9.060	-2.329	15.121	1.00	23.52	C
ATOM	1416	CD	GLU	A	509	-8.971	-0.909	14.578	1.00	30.32	C
ATOM	1417	OE1	GLU	A	509	-8.712	0.038	15.366	1.00	23.83	O
ATOM	1418	OE2	GLU	A	509	-9.139	-0.750	13.346	1.00	24.89	O
ATOM	1419	C	GLU	A	509	-6.954	-3.636	16.829	1.00	24.33	C
ATOM	1420	O	GLU	A	509	-7.196	-4.767	17.246	1.00	24.26	O
ATOM	1421	N	CYS	A	510	-6.009	-3.391	15.913	1.00	20.72	N
ATOM	1422	CA	CYS	A	510	-5.173	-4.456	15.392	1.00	18.85	C
ATOM	1423	CB	CYS	A	510	-4.314	-3.963	14.213	1.00	20.67	C
ATOM	1424	SG	CYS	A	510	-5.287	-3.330	12.822	1.00	25.10	S
ATOM	1425	C	CYS	A	510	-4.216	-4.926	16.503	1.00	21.45	C
ATOM	1426	O	CYS	A	510	-4.026	-6.104	16.720	1.00	24.61	O
ATOM	1427	N	ILE	A	511	-3.590	-3.972	17.164	1.00	22.33	N
ATOM	1428	CA	ILE	A	511	-2.629	-4.304	18.208	1.00	27.31	C
ATOM	1429	CB	ILE	A	511	-1.724	-3.081	18.537	1.00	27.85	C
ATOM	1430	CG2	ILE	A	511	-0.701	-3.445	19.641	1.00	32.87	C
ATOM	1431	CG1	ILE	A	511	-1.004	-2.638	17.255	1.00	27.31	C
ATOM	1432	CD1	ILE	A	511	-0.335	-1.270	17.338	1.00	34.56	C
ATOM	1433	C	ILE	A	511	-3.318	-4.797	19.475	1.00	31.42	C
ATOM	1434	O	ILE	A	511	-2.887	-5.791	20.071	1.00	29.83	O
ATOM	1435	N	ASN	A	512	-4.413	-4.152	19.861	1.00	24.92	N
ATOM	1436	CA	ASN	A	512	-5.068	-4.547	21.093	1.00	27.73	C
ATOM	1437	CB	ASN	A	512	-5.860	-3.387	21.681	1.00	24.36	C
ATOM	1438	CG	ASN	A	512	-4.980	-2.240	22.108	1.00	34.57	C
ATOM	1439	OD1	ASN	A	512	-3.903	-2.442	22.653	1.00	38.07	O
ATOM	1440	ND2	ASN	A	512	-5.447	-1.024	21.872	1.00	38.61	N
ATOM	1441	C	ASN	A	512	-5.973	-5.747	20.953	1.00	30.41	C
ATOM	1442	O	ASN	A	512	-6.100	-6.530	21.893	1.00	30.25	O
ATOM	1443	N	PHE	A	513	-6.622	-5.898	19.804	1.00	23.64	N
ATOM	1444	CA	PHE	A	513	-7.529	-7.031	19.648	1.00	23.12	C
ATOM	1445	CB	PHE	A	513	-8.965	-6.544	19.642	1.00	24.06	C
ATOM	1446	CG	PHE	A	513	-9.365	-5.836	20.901	1.00	33.74	C
ATOM	1447	CD1	PHE	A	513	-9.502	-4.456	20.925	1.00	33.94	C
ATOM	1448	CD2	PHE	A	513	-9.566	-6.558	22.081	1.00	33.20	C
ATOM	1449	CE1	PHE	A	513	-9.829	-3.790	22.119	1.00	40.69	C
ATOM	1450	CE2	PHE	A	513	-9.894	-5.901	23.267	1.00	39.14	C
ATOM	1451	CZ	PHE	A	513	-10.021	-4.517	23.282	1.00	38.17	C
ATOM	1452	C	PHE	A	513	-7.299	-7.940	18.447	1.00	26.12	C
ATOM	1453	O	PHE	A	513	-8.122	-8.815	18.183	1.00	25.90	O
ATOM	1454	N	ARG	A	514	-6.200	-7.719	17.715	1.00	20.92	N
ATOM	1455	CA	ARG	A	514	-5.855	-8.511	16.548	1.00	18.78	C
ATOM	1456	CB	ARG	A	514	-5.504	-9.966	16.974	1.00	22.53	C
ATOM	1457	CG	ARG	A	514	-4.403	-9.980	18.017	1.00	24.16	C

ATOM	1458	CD	ARG	A	514	-3.883	-11.364	18.353	1.00	26.16	C
ATOM	1459	NE	ARG	A	514	-2.727	-11.229	19.247	1.00	25.10	N
ATOM	1460	CZ	ARG	A	514	-1.983	-12.248	19.657	1.00	27.44	C
ATOM	1461	NH1	ARG	A	514	-2.269	-13.477	19.264	1.00	27.42	N
ATOM	1462	NH2	ARG	A	514	-0.928	-12.027	20.443	1.00	29.69	N
ATOM	1463	C	ARG	A	514	-7.008	-8.520	15.532	1.00	19.73	C
ATOM	1464	O	ARG	A	514	-7.173	-9.487	14.790	1.00	21.31	O
ATOM	1465	N	LYS	A	515	-7.733	-7.404	15.480	1.00	22.26	N
ATOM	1466	CA	LYS	A	515	-8.891	-7.277	14.597	1.00	19.38	C
ATOM	1467	CB	LYS	A	515	-9.995	-6.589	15.385	1.00	23.23	C
ATOM	1468	CG	LYS	A	515	-11.303	-6.407	14.627	1.00	24.88	C
ATOM	1469	CD	LYS	A	515	-12.277	-5.554	15.432	1.00	31.97	C
ATOM	1470	CE	LYS	A	515	-13.434	-5.099	14.557	1.00	37.46	C
ATOM	1471	NZ	LYS	A	515	-14.341	-4.148	15.261	1.00	42.53	N
ATOM	1472	C	LYS	A	515	-8.547	-6.460	13.322	1.00	21.36	C
ATOM	1473	O	LYS	A	515	-8.165	-5.303	13.436	1.00	20.92	O
ATOM	1474	N	PHE	A	516	-8.740	-7.059	12.143	1.00	21.89	N
ATOM	1475	CA	PHE	A	516	-8.421	-6.387	10.870	1.00	21.28	C
ATOM	1476	CB	PHE	A	516	-7.346	-7.180	10.127	1.00	20.51	C
ATOM	1477	CG	PHE	A	516	-6.025	-7.215	10.878	1.00	21.58	C
ATOM	1478	CD1	PHE	A	516	-5.857	-8.098	11.954	1.00	23.48	C
ATOM	1479	CD2	PHE	A	516	-4.998	-6.338	10.555	1.00	23.31	C
ATOM	1480	CE1	PHE	A	516	-4.672	-8.099	12.698	1.00	25.88	C
ATOM	1481	CE2	PHE	A	516	-3.814	-6.334	11.296	1.00	24.06	C
ATOM	1482	CZ	PHE	A	516	-3.654	-7.220	12.370	1.00	29.09	C
ATOM	1483	C	PHE	A	516	-9.659	-6.196	10.014	1.00	24.42	C
ATOM	1484	O	PHE	A	516	-10.584	-7.031	10.045	1.00	21.09	O
ATOM	1485	N	SER	A	517	-9.648	-5.111	9.241	1.00	20.69	N
ATOM	1486	CA	SER	A	517	-10.818	-4.718	8.434	1.00	26.64	C
ATOM	1487	CB	SER	A	517	-11.826	-4.042	9.379	1.00	21.54	C
ATOM	1488	OG	SER	A	517	-11.213	-2.897	10.008	1.00	22.44	O
ATOM	1489	C	SER	A	517	-10.377	-3.679	7.393	1.00	21.26	C
ATOM	1490	O	SER	A	517	-9.236	-3.288	7.397	1.00	19.96	O
ATOM	1491	N	SER	A	518	-11.287	-3.223	6.529	1.00	19.99	N
ATOM	1492	CA	SER	A	518	-10.873	-2.180	5.589	1.00	20.05	C
ATOM	1493	CB	SER	A	518	-12.002	-1.884	4.584	1.00	27.16	C
ATOM	1494	OG	SER	A	518	-12.033	-2.959	3.646	1.00	30.81	O
ATOM	1495	C	SER	A	518	-10.473	-0.946	6.366	1.00	19.52	C
ATOM	1496	O	SER	A	518	-9,591	-0.196	5.937	1.00	26.21	O
ATOM	1497	N	ARG	A	519	-11.119	-0.725	7.500	1.00	22.21	N
ATOM	1498	CA	ARG	A	519	-10.780	0.414	8.311	1.00	18.10	C
ATOM	1499	CB	ARG	A	519	-11.842	0.646	9.371	1.00	22.77	C
ATOM	1500	CG	ARG	A	519	-13.023	1.415	8.764	1.00	25.96	C
ATOM	1501	CD	ARG	A	519	-14.180	1.425	9.709	1.00	34.85	C
ATOM	1502	NE	ARG	A	519	-15.279	2.180	9.131	1.00	42.62	N
ATOM	1503	CZ	ARG	A	519	-16.510	2.192	9.633	1.00	49.29	C
ATOM	1504	NH1	ARG	A	519	-16.798	1.484	10.727	1.00	43.62	N
ATOM	1505	NH2	ARG	A	519	-17.458	2.899	9.031	1.00	50.64	N
ATOM	1506	C	ARG	A	519	-9.393	0.343	8.939	1.00	20.79	C
ATOM	1507	O	ARG	A	519	-8.808	1.403	9.221	1.00	20.53	O
ATOM	1508	N	SER	A	520	-8.877	-0.867	9.182	1.00	18.48	N
ATOM	1509	CA	SER	A	520	-7.508	-0.904	9.705	1.00	19.17	C
ATOM	1510	CB	SER	A	520	-7.177	-2.264	10.410	1.00	17.39	C
ATOM	1511	OG	SER	A	520	-7.348	-3.401	9.603	1.00	22.96	O
ATOM	1512	C	SER	A	520	-6.586	-0.607	8.484	1.00	18.94	C
ATOM	1513	O	SER	A	520	-5.506	-0.023	8.631	1.00	21.65	O
ATOM	1514	N	ASP	A	521	-7.032	-0.960	7.272	1.00	19.22	N
ATOM	1515	CA	ASP	A	521	-6.261	-0.657	6.038	1.00	23.13	C
ATOM	1516	CB	ASP	A	521	-6.902	-1.257	4.770	1.00	27.96	C
ATOM	1517	CG	ASP	A	521	-6.488	-2.716	4.501	1.00	23.02	C
ATOM	1518	OD1	ASP	A	521	-5.536	-3.223	5.145	1.00	22.00	O
ATOM	1519	OD2	ASP	A	521	-7.113	-3.347	3.598	1.00	23.07	O
ATOM	1520	C	ASP	A	521	-6.253	0.877	5.874	1.00	18.27	C
ATOM	1521	O	ASP	A	521	-5.238	1.473	5.445	1.00	20.55	O
ATOM	1522	N	VAL	A	522	-7.366	1.525	6.246	1.00	16.95	N
ATOM	1523	CA	VAL	A	522	-7.421	3.004	6.168	1.00	16.30	C
ATOM	1524	CB	VAL	A	522	-8.833	3.534	6.537	1.00	18.70	C
ATOM	1525	CG1	VAL	A	522	-8.820	5.066	6.757	1.00	19.08	C

ATOM	1526	CG2	VAL	A	522	-9.801	3.174	5.395	1.00 15.77	C
ATOM	1527	C	VAL	A	522	-6.361	3.620	7.093	1.00 20.10	C
ATOM	1528	O	VAL	A	522	-5.670	4.569	6.711	1.00 19.37	O
ATOM	1529	N	TRP	A	523	-6.210	3.069	8.294	1.00 19.01	N
ATOM	1530	CA	TRP	A	523	-5.186	3.593	9.216	1.00 17.00	C
ATOM	1531	CB	TRP	A	523	-5.240	2.819	10.551	1.00 16.75	C
ATOM	1532	CG	TRP	A	523	-4.247	3.339	11.594	1.00 17.47	C
ATOM	1533	CD2	TRP	A	523	-4.561	4.078	12.781	1.00 18.40	C
ATOM	1534	CE2	TRP	A	523	-3.336	4.384	13.411	1.00 19.18	C
ATOM	1535	CE3	TRP	A	523	-5.763	4.514	13.379	1.00 16.68	C
ATOM	1536	CD1	TRP	A	523	-2.889	3.226	11.559	1.00 22.45	C
ATOM	1537	NE1	TRP	A	523	-2.327	3.856	12.650	1.00 17.34	N
ATOM	1538	CZ2	TRP	A	523	-3.267	5.112	14.607	1.00 20.28	C
ATOM	1539	CZ3	TRP	A	523	-5.692	5.242	14.570	1.00 18.90	C
ATOM	1540	CH2	TRP	A	523	-4.457	5.536	15.170	1.00 20.73	C
ATOM	1541	C	TRP	A	523	-3.799	3.464	8.573	1.00 16.27	C
ATOM	1542	O	TRP	A	523	-2.988	4.402	8.628	1.00 19.33	O
ATOM	1543	N	SER	A	524	-3.528	2.315	7.952	1.00 17.09	N
ATOM	1544	CA	SER	A	524	-2.231	2.082	7.277	1.00 22.19	C
ATOM	1545	CB	SER	A	524	-2.178	0.658	6.722	1.00 21.77	C
ATOM	1546	OG	SER	A	524	-2.247	-0.299	7.751	1.00 31.82	O
ATOM	1547	C	SER	A	524	-2.008	3.039	6.114	1.00 23.32	C
ATOM	1548	O	SER	A	524	-0.888	3.499	5.878	1.00 17.77	O
ATOM	1549	N	TYR	A	525	-3.076	3.334	5.381	1.00 22.60	N
ATOM	1550	CA	TYR	A	525	-3.042	4.279	4.274	1.00 22.61	C
ATOM	1551	CB	TYR	A	525	-4.457	4.413	3.642	1.00 20.36	C
ATOM	1552	CG	TYR	A	525	-4.463	5.402	2.506	1.00 18.97	C
ATOM	1553	CD1	TYR	A	525	-3.886	5.077	1.285	1.00 21.53	C
ATOM	1554	CE1	TYR	A	525	-3.835	6.020	0.230	1.00 20.51	C
ATOM	1555	CD2	TYR	A	525	-5.005	6.685	2.673	1.00 20.00	C
ATOM	1556	CE2	TYR	A	525	-4.961	7.620	1.642	1.00 21.87	C
ATOM	1557	CZ	TYR	A	525	-4.376	7.284	0.428	1.00 24.64	C
ATOM	1558	OH	TYR	A	525	-4.358	8.214	-0.589	1.00 24.81	O
ATOM	1559	C	TYR	A	525	-2.590	5.634	4.815	1.00 18.79	C
ATOM	1560	O	TYR	A	525	-1.760	6.319	4.208	1.00 22.11	O
ATOM	1561	N	GLY	A	526	-3.133	6.036	5.963	1.00 16.47	N
ATOM	1562	CA	GLY	A	526	-2.737	7.291	6.582	1.00 17.93	C
ATOM	1563	C	GLY	A	526	-1.233	7.343	6.852	1.00 20.82	C
ATOM	1564	O	GLY	A	526	-0.571	8.366	6.583	1.00 20.21	O
ATOM	1565	N	VAL	A	527	-0.691	6.262	7.409	1.00 18.53	N
ATOM	1566	CA	VAL	A	527	0.755	6.202	7.680	1.00 15.75	C
ATOM	1567	CB	VAL	A	527	1.109	4.902	8.447	1.00 20.06	C
ATOM	1568	CG1	VAL	A	527	2.624	4.842	8.768	1.00 18.66	C
ATOM	1569	CG2	VAL	A	527	0.292	4.872	9.769	1.00 19.72	C
ATOM	1570	C	VAL	A	527	1.490	6.249	6.326	1.00 16.40	C
ATOM	1571	O	VAL	A	527	2.527	6.888	6.205	1.00 21.73	O
ATOM	1572	N	THR	A	528	0.941	5.594	5.307	1.00 19.11	N
ATOM	1573	CA	THR	A	528	1.562	5.595	3.975	1.00 18.53	C
ATOM	1574	CB	THR	A	528	0.794	4.663	3.020	1.00 21.20	C
ATOM	1575	OG1	THR	A	528	0.891	3.318	3.519	1.00 21.69	O
ATOM	1576	CG2	THR	A	528	1.392	4.705	1.618	1.00 22.45	C
ATOM	1577	C	THR	A	528	1.587	7.032	3.416	1.00 24.70	C
ATOM	1578	O	THR	A	528	2.599	7.456	2.850	1.00 19.73	O
ATOM	1579	N	MET	A	529	0.479	7.764	3.587	1.00 19.61	N
ATOM	1580	CA	MET	A	529	0.425	9.179	3.143	1.00 19.25	C
ATOM	1581	CB	MET	A	529	-0.902	9.848	3.576	1.00 20.84	C
ATOM	1582	CG	MET	A	529	-2.135	9.296	2.846	1.00 22.24	C
ATOM	1583	SD	MET	A	529	-3.608	10.284	3.352	1.00 24.00	S
ATOM	1584	CE	MET	A	529	-3.207	11.921	2.622	1.00 23.54	C
ATOM	1585	C	MET	A	529	1.560	9.943	3.821	1.00 19.48	C
ATOM	1586	O	MET	A	529	2.276	10.736	3.182	1.00 20.92	O
ATOM	1587	N	TRP	A	530	1.724	9.726	5.124	1.00 19.75	N
ATOM	1588	CA	TRP	A	530	2.777	10.434	5.882	1.00 18.54	C
ATOM	1589	CB	TRP	A	530	2.731	10.069	7.376	1.00 20.48	C
ATOM	1590	CG	TRP	A	530	3.582	10.944	8.225	1.00 18.20	C
ATOM	1591	CD2	TRP	A	530	4.969	10.745	8.527	1.00 18.21	C
ATOM	1592	CE2	TRP	A	530	5.389	11.838	9.336	1.00 19.74	C
ATOM	1593	CE3	TRP	A	530	5.899	9.752	8.197	1.00 20.68	C

ATOM	1594	CD1	TRP	A	530	3.214	12.116	8.842	1.00	18.28	C
ATOM	1595	NE1	TRP	A	530	4.305	12.661	9.520	1.00	22.22	N
ATOM	1596	CZ2	TRP	A	530	6.712	11.961	9.819	1.00	25.36	C
ATOM	1597	CZ3	TRP	A	530	7.212	9.872	8.681	1.00	22.68	C
ATOM	1598	CH2	TRP	A	530	7.598	10.969	9.479	1.00	26.97	C
ATOM	1599	C	TRP	A	530	4.171	10.152	5.349	1.00	21.37	C
ATOM	1600	O	TRP	A	530	4.972	11.093	5.118	1.00	22.21	O
ATOM	1601	N	GLU	A	531	4.475	8.870	5.161	1.00	22.41	N
ATOM	1602	CA	GLU	A	531	5.773	8.443	4.634	1.00	23.01	C
ATOM	1603	CB	GLU	A	531	5.800	6.938	4.345	1.00	22.19	C
ATOM	1604	CG	GLU	A	531	5.636	5.990	5.540	1.00	26.83	C
ATOM	1605	CD	GLU	A	531	5.699	4.530	5.079	1.00	29.43	C
ATOM	1606	OE1	GLU	A	531	4.621	3.926	4.848	1.00	23.48	O
ATOM	1607	OE2	GLU	A	531	6.836	3.999	4.921	1.00	26.99	O
ATOM	1608	C	GLU	A	531	6.035	9.114	3.304	1.00	22.15	C
ATOM	1609	O	GLU	A	531	7.149	9.587	3.030	1.00	22.47	O
ATOM	1610	N	ALA	A	532	5.017	9.120	2.445	1.00	20.60	N
ATOM	1611	CA	ALA	A	532	5.170	9.710	1.121	1.00	20.49	C
ATOM	1612	CB	ALA	A	532	3.951	9.366	0.222	1.00	21.29	C
ATOM	1613	C	ALA	A	532	5.376	11.209	1.143	1.00	22.68	C
ATOM	1614	O	ALA	A	532	6.294	11.721	0.487	1.00	21.66	O
ATOM	1615	N	LEU	A	533	4.523	11.918	1.881	1.00	24.52	N
ATOM	1616	CA	LEU	A	533	4.601	13.377	1.957	1.00	27.55	C
ATOM	1617	CB	LEU	A	533	3.301	13.951	2.553	1.00	23.33	C
ATOM	1618	CG	LEU	A	533	2.113	13.809	1.586	1.00	24.16	C
ATOM	1619	CD1	LEU	A	533	0.784	14.069	2.314	1.00	30.47	C
ATOM	1620	CD2	LEU	A	533	2.289	14.808	0.408	1.00	26.48	C
ATOM	1621	C	LEU	A	533	5.832	13.849	2.737	1.00	28.49	C
ATOM	1622	O	LEU	A	533	6.213	15.021	2.661	1.00	23.09	O
ATOM	1623	N	SER	A	534	6.458	12.921	3.462	1.00	23.64	N
ATOM	1624	CA	SER	A	534	7.686	13.216	4.218	1.00	24.10	C
ATOM	1625	CB	SER	A	534	7.717	12.409	5.509	1.00	24.84	C
ATOM	1626	OG	SER	A	534	6.724	12.875	6.402	1.00	32.38	O
ATOM	1627	C	SER	A	534	8.867	12.778	3.370	1.00	23.66	C
ATOM	1628	O	SER	A	534	10.004	12.749	3.839	1.00	26.17	O
ATOM	1629	N	TYR	A	535	8.581	12.408	2.130	1.00	23.34	N
ATOM	1630	CA	TYR	A	535	9.593	11.943	1.196	1.00	28.19	C
ATOM	1631	CB	TYR	A	535	10.485	13.112	0.733	1.00	28.89	C
ATOM	1632	CG	TYR	A	535	9.724	14.020	-0.219	1.00	29.59	C
ATOM	1633	CD1	TYR	A	535	8.811	14.939	0.274	1.00	28.98	C
ATOM	1634	CE1	TYR	A	535	8.026	15.712	-0.584	1.00	30.80	C
ATOM	1635	CD2	TYR	A	535	9.849	13.887	-1.599	1.00	26.41	C
ATOM	1636	CE2	TYR	A	535	9.063	14.647	-2.472	1.00	29.12	C
ATOM	1637	CZ	TYR	A	535	8.155	15.558	-1.948	1.00	23.83	C
ATOM	1638	OH	TYR	A	535	7.383	16.325	-2.773	1.00	30.19	O
ATOM	1639	C	TYR	A	535	10.447	10.781	1.709	1.00	32.28	C
ATOM	1640	O	TYR	A	535	11.672	10.845	1.691	1.00	27.48	O
ATOM	1641	N	GLY	A	536	9.781	9.722	2.174	1.00	26.27	N
ATOM	1642	CA	GLY	A	536	10.495	8.530	2.610	1.00	25.77	C
ATOM	1643	C	GLY	A	536	11.019	8.433	4.022	1.00	30.26	C
ATOM	1644	O	GLY	A	536	11.754	7.499	4.353	1.00	37.11	O
ATOM	1645	N	GLN	A	537	10.648	9.380	4.876	1.00	30.46	N
ATOM	1646	CA	GLN	A	537	11.080	9.346	6.263	1.00	28.08	C
ATOM	1647	CB	GLN	A	537	10.740	10.672	6.935	1.00	34.05	C
ATOM	1648	CG	GLN	A	537	11.750	11.776	6.618	1.00	44.08	C
ATOM	1649	CD	GLN	A	537	11.367	13.123	7.203	1.00	46.85	C
ATOM	1650	OE1	GLN	A	537	10.983	13.224	8.371	1.00	55.73	O
ATOM	1651	NE2	GLN	A	537	11.477	14.170	6.394	1.00	50.81	N
ATOM	1652	C	GLN	A	537	10.401	8.188	7.011	1.00	29.96	C
ATOM	1653	O	GLN	A	537	9.343	7.715	6.601	1.00	24.20	O
ATOM	1654	N	LYS	A	538	11.028	7.722	8.094	1.00	26.82	N
ATOM	1655	CA	LYS	A	538	10.446	6.638	8.870	1.00	27.30	C
ATOM	1656	CB	LYS	A	538	11.533	5.871	9.635	1.00	32.27	C
ATOM	1657	CG	LYS	A	538	12.495	5.132	8.724	1.00	41.48	C
ATOM	1658	CD	LYS	A	538	13.536	4.359	9.529	1.00	46.01	C
ATOM	1659	CE	LYS	A	538	14.278	3.365	8.644	1.00	48.76	C
ATOM	1660	NZ	LYS	A	538	15.278	2.577	9.429	1.00	54.95	N
ATOM	1661	C	LYS	A	538	9.431	7.175	9.875	1.00	28.24	C

ATOM	1662	O	LYS	A	538	9.665	8.195	10.529	1.00	28.85	O
ATOM	1663	N	PRO	A	539	8.283	6.496	10.008	1.00	24.53	N
ATOM	1664	CD	PRO	A	539	7.742	5.389	9.198	1.00	22.29	C
ATOM	1665	CA	PRO	A	539	7.286	6.966	10.972	1.00	24.04	C
ATOM	1666	CB	PRO	A	539	6.053	6.118	10.644	1.00	28.10	C
ATOM	1667	CG	PRO	A	539	6.644	4.857	10.098	1.00	36.04	C
ATOM	1668	C	PRO	A	539	7.737	6.759	12.421	1.00	28.35	C
ATOM	1669	O	PRO	A	539	8.426	5.783	12.734	1.00	25.90	O
ATOM	1670	N	TYR	A	540	7.343	7.680	13.292	1.00	23.53	N
ATOM	1671	CA	TYR	A	540	7.656	7.645	14.722	1.00	28.38	C
ATOM	1672	CB	TYR	A	540	6.831	6.555	15.418	1.00	24.00	C
ATOM	1673	CG	TYR	A	540	5.331	6.586	15.095	1.00	27.38	C
ATOM	1674	CD1	TYR	A	540	4.477	7.452	15.766	1.00	24.16	C
ATOM	1675	CE1	TYR	A	540	3.096	7.476	15.483	1.00	20.41	C
ATOM	1676	CD2	TYR	A	540	4.800	5.746	14.119	1.00	28.23	C
ATOM	1677	CE2	TYR	A	540	3.417	5.767	13.800	1.00	21.95	C
ATOM	1678	CZ	TYR	A	540	2.580	6.632	14.496	1.00	20.01	C
ATOM	1679	OH	TYR	A	540	1.244	6.670	14.207	1.00	24.93	O
ATOM	1680	C	TYR	A	540	9.136	7.346	14.903	1.00	28.93	C
ATOM	1681	O	TYR	A	540	9.508	6.478	15.689	1.00	30.14	O
ATOM	1682	N	LYS	A	541	9.942	8.095	14.152	1.00	27.25	N
ATOM	1683	CA	LYS	A	541	11.391	7.985	14.100	1.00	39.82	C
ATOM	1684	CB	LYS	A	541	11.939	9.274	13.472	1.00	44.06	C
ATOM	1685	CG	LYS	A	541	13.334	9.167	12.893	1.00	54.68	C
ATOM	1686	CD	LYS	A	541	13.699	10.418	12.075	1.00	54.79	C
ATOM	1687	CE	LYS	A	541	12.794	10.586	10.848	1.00	59.69	C
ATOM	1688	NZ	LYS	A	541	13.234	11.695	9.938	1.00	56.19	N
ATOM	1689	C	LYS	A	541	12.074	7.722	15.447	1.00	42.70	C
ATOM	1690	O	LYS	A	541	12.849	6.777	15.590	1.00	43.82	O
ATOM	1691	N	LYS	A	542	11.784	8.549	16.433	1.00	44.10	N
ATOM	1692	CA	LYS	A	542	12.425	8.378	17.728	1.00	51.64	C
ATOM	1693	CB	LYS	A	542	12.682	9.749	18.350	1.00	51.94	C
ATOM	1694	CG	LYS	A	542	11.425	10.565	18.581	1.00	56.75	C
ATOM	1695	CD	LYS	A	542	11.731	11.841	19.359	1.00	59.67	C
ATOM	1696	CE	LYS	A	542	10.445	12.559	19.767	1.00	60.04	C
ATOM	1697	NZ	LYS	A	542	10.684	13.819	20.538	1.00	63.82	N
ATOM	1698	C	LYS	A	542	11.649	7.512	18.709	1.00	55.84	C
ATOM	1699	O	LYS	A	542	11.746	7.724	19.920	1.00	59.11	O
ATOM	1700	N	MET	A	543	10.908	6.523	18.207	1.00	41.98	N
ATOM	1701	CA	MET	A	543	10.125	5.658	19.083	1.00	43.90	C
ATOM	1702	CB	MET	A	543	8.645	6.029	19.019	1.00	45.70	C
ATOM	1703	CG	MET	A	543	8.230	7.209	19.856	1.00	53.80	C
ATOM	1704	SD	MET	A	543	6.477	7.548	19.578	1.00	44.32	S
ATOM	1705	CE	MET	A	543	6.609	9.128	18.721	1.00	44.97	C
ATOM	1706	C	MET	A	543	10.235	4.185	18.755	1.00	46.16	C
ATOM	1707	O	MET	A	543	10.497	3.805	17.616	1.00	49.81	O
ATOM	1708	N	LYS	A	544	10.001	3.359	19.769	1.00	48.84	N
ATOM	1709	CA	LYS	A	544	10.042	1.909	19.627	1.00	54.57	C
ATOM	1710	CB	LYS	A	544	10.872	1.284	20.748	1.00	54.75	C
ATOM	1711	CG	LYS	A	544	10.262	1.451	22.134	1.00	63.19	C
ATOM	1712	CD	LYS	A	544	11.076	0.704	23.191	1.00	63.73	C
ATOM	1713	CE	LYS	A	544	10.400	0.726	24.560	1.00	65.53	C
ATOM	1714	NZ	LYS	A	544	11.146	-0.103	25.561	1.00	62.21	N
ATOM	1715	C	LYS	A	544	8.612	1.374	19.699	1.00	57.82	C
ATOM	1716	O	LYS	A	544	7.655	2.112	19.464	1.00	56.73	O
ATOM	1717	N	GLY	A	545	8.475	0.096	20.046	1.00	53.41	N
ATOM	1718	CA	GLY	A	545	7.161	-0.512	20.128	1.00	51.20	C
ATOM	1719	C	GLY	A	545	6.218	0.124	21.133	1.00	51.82	C
ATOM	1720	O	GLY	A	545	5.359	0.915	20.752	1.00	53.88	O
ATOM	1721	N	PRO	A	546	6.350	-0.206	22.427	1.00	52.05	N
ATOM	1722	CD	PRO	A	546	7.333	-1.165	22.966	1.00	55.28	C
ATOM	1723	CA	PRO	A	546	5.507	0.321	23.506	1.00	51.30	C
ATOM	1724	CB	PRO	A	546	6.215	-0.181	24.768	1.00	52.03	C
ATOM	1725	CG	PRO	A	546	6.743	-1.503	24.322	1.00	51.79	C
ATOM	1726	C	PRO	A	546	5.325	1.835	23.515	1.00	44.10	C
ATOM	1727	O	PRO	A	546	4.296	2.342	23.983	1.00	37.86	O
ATOM	1728	N	GLU	A	547	6.329	2.553	23.017	1.00	39.18	N
ATOM	1729	CA	GLU	A	547	6.274	4.004	22.973	1.00	45.81	C

ATOM	1730	CB	GLU	A	547	7.607	4.582	22.516	1.00	44.80	C
ATOM	1731	CG	GLU	A	547	8.760	4.296	23.450	1.00	60.26	C
ATOM	1732	CD	GLU	A	547	10.033	4.970	23.001	1.00	56.95	C
ATOM	1733	OE1	GLU	A	547	10.093	6.220	23.034	1.00	61.75	O
ATOM	1734	OE2	GLU	A	547	10.970	4.247	22.608	1.00	59.24	O
ATOM	1735	C	GLU	A	547	5.173	4.495	22.030	1.00	31.92	C
ATOM	1736	O	GLU	A	547	4.417	5.381	22.384	1.00	33.88	O
ATOM	1737	N	VAL	A	548	5.113	3.922	20.834	1.00	36.76	N
ATOM	1738	CA	VAL	A	548	4.097	4.331	19.849	1.00	30.35	C
ATOM	1739	CB	VAL	A	548	4.316	3.610	18.513	1.00	35.20	C
ATOM	1740	CG1	VAL	A	548	3.289	4.083	17.486	1.00	31.70	C
ATOM	1741	CG2	VAL	A	548	5.723	3.888	18.016	1.00	39.20	C
ATOM	1742	C	VAL	A	548	2.678	4.060	20.344	1.00	32.59	C
ATOM	1743	O	VAL	A	548	1.801	4.913	20.242	1.00	32.29	O
ATOM	1744	N	MET	A	549	2.448	2.874	20.899	1.00	34.32	N
ATOM	1745	CA	MET	A	549	1.131	2.528	21.418	1.00	33.89	C
ATOM	1746	CB	MET	A	549	1.171	1.125	22.025	1.00	43.40	C
ATOM	1747	CG	MET	A	549	-0.202	0.486	22.120	1.00	54.00	C
ATOM	1748	SD	MET	A	549	-1.061	0.474	20.506	1.00	73.10	S
ATOM	1749	CE	MET	A	549	-2.239	1.839	20.656	1.00	53.85	C
ATOM	1750	C	MET	A	549	0.650	3.532	22.476	1.00	31.82	C
ATOM	1751	O	MET	A	549	-0.486	4.000	22.436	1.00	30.85	O
ATOM	1752	N	ALA	A	550	1.525	3.856	23.420	1.00	30.61	N
ATOM	1753	CA	ALA	A	550	1.194	4.791	24.490	1.00	32.54	C
ATOM	1754	CB	ALA	A	550	2.363	4.852	25.488	1.00	37.38	C
ATOM	1755	C	ALA	A	550	0.910	6.186	23.911	1.00	27.78	C
ATOM	1756	O	ALA	A	550	0.004	6.894	24.362	1.00	28.75	O
ATOM	1757	N	PHE	A	551	1.711	6.569	22.920	1.00	26.75	N
ATOM	1758	CA	PHE	A	551	1.595	7.861	22.220	1.00	29.08	C
ATOM	1759	CB	PHE	A	551	2.712	7.922	21.157	1.00	21.20	C
ATOM	1760	CG	PHE	A	551	2.791	9.219	20.382	1.00	25.99	C
ATOM	1761	CD1	PHE	A	551	3.346	10.358	20.954	1.00	30.16	C
ATOM	1762	CD2	PHE	A	551	2.370	9.265	19.041	1.00	29.19	C
ATOM	1763	CE1	PHE	A	551	3.497	11.540	20.206	1.00	26.26	C
ATOM	1764	CE2	PHE	A	551	2.521	10.449	18.286	1.00	24.90	C
ATOM	1765	CZ	PHE	A	551	3.087	11.577	18.877	1.00	28.07	C
ATOM	1766	C	PHE	A	551	0.214	7.955	21.565	1.00	23.03	C
ATOM	1767	O	PHE	A	551	-0.516	8.922	21.748	1.00	24.86	O
ATOM	1768	N	ILE	A	552	-0.149	6.931	20.806	1.00	23.91	N
ATOM	1769	CA	ILE	A	552	-1.452	6.917	20.145	1.00	23.84	C
ATOM	1770	CB	ILE	A	552	-1.559	5.675	19.241	1.00	24.60	C
ATOM	1771	CG2	ILE	A	552	-2.973	5.513	18.716	1.00	26.02	C
ATOM	1772	CG1	ILE	A	552	-0.476	5.757	18.155	1.00	28.63	C
ATOM	1773	CD1	ILE	A	552	-0.614	6.952	17.164	1.00	28.18	C
ATOM	1774	C	ILE	A	552	-2.575	6.921	21.184	1.00	24.71	C
ATOM	1775	O	ILE	A	552	-3.565	7.653	21.048	1.00	25.03	O
ATOM	1776	N	GLU	A	553	-2.419	6.121	22.238	1.00	26.97	N
ATOM	1777	CA	GLU	A	553	-3.433	6.055	23.295	1.00	27.80	C
ATOM	1778	CB	GLU	A	553	-3.040	5.014	24.346	1.00	39.68	C
ATOM	1779	CG	GLU	A	553	-3.089	3.573	23.834	1.00	47.86	C
ATOM	1780	CD	GLU	A	553	-4.506	3.085	23.586	1.00	47.67	C
ATOM	1781	OE1	GLU	A	553	-4.662	2.019	22.950	1.00	54.95	O
ATOM	1782	OE2	GLU	A	553	-5.460	3.758	24.032	1.00	55.56	O
ATOM	1783	C	GLU	A	553	-3.645	7.424	23.972	1.00	27.09	C
ATOM	1784	O	GLU	A	553	-4.757	7.751	24.386	1.00	33.91	O
ATOM	1785	N	GLN	A	554	-2.577	8.206	24.088	1.00	30.97	N
ATOM	1786	CA	GLN	A	554	-2.639	9.545	24.678	1.00	31.06	C
ATOM	1787	CB	GLN	A	554	-1.232	10.093	24.909	1.00	33.93	C
ATOM	1788	CG	GLN	A	554	-0.454	9.441	26.030	1.00	47.13	C
ATOM	1789	CD	GLN	A	554	0.949	9.978	26.069	1.00	48.57	C
ATOM	1790	OE1	GLN	A	554	1.159	11.187	25.932	1.00	53.53	O
ATOM	1791	NE2	GLN	A	554	1.921	9.089	26.250	1.00	53.00	N
ATOM	1792	C	GLN	A	554	-3.364	10.534	23.767	1.00	34.15	C
ATOM	1793	O	GLN	A	554	-3.599	11.677	24.155	1.00	29.68	O
ATOM	1794	N	GLY	A	555	-3.698	10.104	22.552	1.00	28.32	N
ATOM	1795	CA	GLY	A	555	-4.389	11.008	21.644	1.00	30.45	C
ATOM	1796	C	GLY	A	555	-3.449	11.876	20.805	1.00	27.04	C
ATOM	1797	O	GLY	A	555	-3.859	12.914	20.269	1.00	28.32	O

ATOM	1798	N	LYS	A	556	-2.188	11.478	20.694	1.00 21.48	N
ATOM	1799	CA	LYS	A	556	-1.240	12.239	19.886	1.00 21.96	C
ATOM	1800	CB	LYS	A	556	0.096	12.390	20.618	1.00 22.25	C
ATOM	1801	CG	LYS	A	556	-0.048	13.123	21.964	1.00 24.42	C
ATOM	1802	CD	LYS	A	556	1.312	13.380	22.586	1.00 25.86	C
ATOM	1803	CE	LYS	A	556	1.157	14.112	23.934	1.00 34.77	C
ATOM	1804	NZ	LYS	A	556	2.485	14.453	24.554	1.00 33.67	N
ATOM	1805	C	LYS	A	556	-1.007	11.516	18.567	1.00 23.68	C
ATOM	1806	O	LYS	A	556	-1.140	10.291	18.492	1.00 22.12	O
ATOM	1807	N	ARG	A	557	-0.610	12.285	17.548	1.00 19.92	N
ATOM	1808	CA	ARG	A	557	-0.365	11.722	16.229	1.00 20.32	C
ATOM	1809	CB	ARG	A	557	-1.575	11.983	15.311	1.00 20.48	C
ATOM	1810	CG	ARG	A	557	-2.895	11.354	15.818	1.00 21.21	C
ATOM	1811	CD	ARG	A	557	-2.900	9.812	15.730	1.00 19.93	C
ATOM	1812	NE	ARG	A	557	-4.203	9.222	16.106	1.00 19.69	N
ATOM	1813	CZ	ARG	A	557	-4.580	8.900	17.343	1.00 22.33	C
ATOM	1814	NH1	ARG	A	557	-3.755	9.098	18.397	1.00 21.75	N
ATOM	1815	NH2	ARG	A	557	-5.771	8.337	17.536	1.00 19.39	N
ATOM	1816	C	ARG	A	557	0.890	12.335	15.616	1.00 20.01	C
ATOM	1817	O	ARG	A	557	1.419	13.342	16.131	1.00 21.06	O
ATOM	1818	N	MET	A	558	1.371	11.729	14.526	1.00 23.13	N
ATOM	1819	CA	MET	A	558	2.562	12.260	13.862	1.00 24.90	C
ATOM	1820	CB	MET	A	558	2.999	11.351	12.710	1.00 20.87	C
ATOM	1821	CG	MET	A	558	3.673	10.070	13.153	1.00 26.00	C
ATOM	1822	SD	MET	A	558	4.400	9.177	11.757	1.00 25.21	S
ATOM	1823	CE	MET	A	558	2.987	8.458	10.949	1.00 19.49	C
ATOM	1824	C	MET	A	558	2.287	13.669	13.330	1.00 27.66	C
ATOM	1825	O	MET	A	558	1.164	13.992	12.898	1.00 21.51	O
ATOM	1826	N	GLU	A	559	3.321	14.503	13.371	1.00 24.36	N
ATOM	1827	CA	GLU	A	559	3.230	15.871	12.908	1.00 26.80	C
ATOM	1828	CB	GLU	A	559	4.539	16.613	13.219	1.00 33.66	C
ATOM	1829	CG	GLU	A	559	5.822	15.788	12.977	1.00 43.05	C
ATOM	1830	CD	GLU	A	559	6.068	14.712	14.060	1.00 54.97	C
ATOM	1831	OE1	GLU	A	559	6.463	15.072	15.198	1.00 59.07	O
ATOM	1832	OE2	GLU	A	559	5.867	13.506	13.774	1.00 44.76	O
ATOM	1833	C	GLU	A	559	2.939	15.992	11.417	1.00 27.49	C
ATOM	1834	O	GLU	A	559	3.209	15.088	10.642	1.00 27.65	O
ATOM	1835	N	CYS	A	560	2.387	17.130	11.026	1.00 22.31	N
ATOM	1836	CA	CYS	A	560	2.122	17.377	9.616	1.00 23.70	C
ATOM	1837	CB	CYS	A	560	1.293	18.655	9.468	1.00 27.79	C
ATOM	1838	SG	CYS	A	560	0.980	19.104	7.751	1.00 30.84	S
ATOM	1839	C	CYS	A	560	3.490	17.535	8.905	1.00 29.44	C
ATOM	1840	O	CYS	A	560	4.350	18.300	9.351	1.00 29.36	O
ATOM	1841	N	PRO	A	561	3.733	16.769	7.825	1.00 29.57	N
ATOM	1842	CD	PRO	A	561	2.944	15.629	7.312	1.00 26.67	C
ATOM	1843	CA	PRO	A	561	5.018	16.890	7.116	1.00 31.79	C
ATOM	1844	CB	PRO	A	561	4.865	15.932	5.933	1.00 29.22	C
ATOM	1845	CG	PRO	A	561	3.976	14.837	6.496	1.00 25.42	C
ATOM	1846	C	PRO	A	561	5.244	18.319	6.619	1.00 29.76	C
ATOM	1847	O	PRO	A	561	4.302	19.055	6.362	1.00 26.53	O
ATOM	1848	N	PRO	A	562	6.502	18.728	6.473	1.00 36.98	N
ATOM	1849	CD	PRO	A	562	7.740	18.045	6.884	1.00 38.45	C
ATOM	1850	CA	PRO	A	562	6.775	20.085	5.994	1.00 38.46	C
ATOM	1851	CB	PRO	A	562	8.302	20.140	5.984	1.00 42.62	C
ATOM	1852	CG	PRO	A	562	8.674	19.202	7.102	1.00 47.24	C
ATOM	1853	C	PRO	A	562	6.177	20.293	4.596	1.00 36.90	C
ATOM	1854	O	PRO	A	562	6.268	19.415	3.745	1.00 37.38	O
ATOM	1855	N	GLU	A	563	5.550	21.445	4.363	1.00 38.19	N
ATOM	1856	CA	GLU	A	563	4.968	21.740	3.048	1.00 43.57	C
ATOM	1857	CB	GLU	A	563	6.025	21.554	1.944	1.00 50.62	C
ATOM	1858	CG	GLU	A	563	7.282	22.401	2.118	1.00 53.80	C
ATOM	1859	CD	GLU	A	563	8.502	21.788	1.429	1.00 62.44	C
ATOM	1860	OE1	GLU	A	563	8.457	21.580	0.193	1.00 63.21	O
ATOM	1861	OE2	GLU	A	563	9.504	21.509	2.131	1.00 64.48	O
ATOM	1862	C	GLU	A	563	3.720	20.924	2.698	1.00 44.24	C
ATOM	1863	O	GLU	A	563	3.164	21.068	1.607	1.00 48.48	O
ATOM	1864	N	CYS	A	564	3.275	20.048	3.598	1.00 41.39	N
ATOM	1865	CA	CYS	A	564	2.060	19.285	3.344	1.00 37.90	C

ATOM	1866	CB	CYS	A	564	1.968	18.064	4.279	1.00	37.32	C
ATOM	1867	SG	CYS	A	564	0.438	17.119	4.110	1.00	38.37	S
ATOM	1868	C	CYS	A	564	0.884	20.221	3.602	1.00	37.50	C
ATOM	1869	O	CYS	A	564	0.753	20.773	4.698	1.00	38.57	O
ATOM	1870	N	PRO	A	565	0.012	20.416	2.597	1.00	37.07	N
ATOM	1871	CD	PRO	A	565	0.058	19.780	1.271	1.00	42.57	C
ATOM	1872	CA	PRO	A	565	-1.160	21.294	2.716	1.00	33.51	C
ATOM	1873	CB	PRO	A	565	-1.791	21.231	1.330	1.00	40.30	C
ATOM	1874	CG	PRO	A	565	-1.369	19.883	0.824	1.00	44.48	C
ATOM	1875	C	PRO	A	565	-2.114	20.827	3.792	1.00	35.24	C
ATOM	1876	O	PRO	A	565	-2.258	19.622	4.024	1.00	32.71	O
ATOM	1877	N	PRO	A	566	-2.800	21.776	4.448	1.00	34.52	N
ATOM	1878	CD	PRO	A	566	-2.692	23.231	4.207	1.00	34.66	C
ATOM	1879	CA	PRO	A	566	-3.762	21.487	5.516	1.00	30.97	C
ATOM	1880	CB	PRO	A	566	-4.398	22.862	5.795	1.00	34.13	C
ATOM	1881	CG	PRO	A	566	-3.308	23.823	5.454	1.00	32.16	C
ATOM	1882	C	PRO	A	566	-4.814	20.438	5.135	1.00	34.26	C
ATOM	1883	O	PRO	A	566	-5.149	19.585	5.950	1.00	28.40	O
ATOM	1884	N	GLU	A	567	-5.331	20.498	3.902	1.00	27.60	N
ATOM	1885	CA	GLU	A	567	-6.367	19.562	3.456	1.00	32.42	C
ATOM	1886	CB	GLU	A	567	-6.859	19.918	2.036	1.00	36.27	C
ATOM	1887	CG	GLU	A	567	-6.961	21.413	1.739	1.00	49.38	C
ATOM	1888	CD	GLU	A	567	-5.604	22.059	1.539	1.00	48.16	C
ATOM	1889	OE1	GLU	A	567	-4.880	21.658	0.602	1.00	63.97	O
ATOM	1890	OE2	GLU	A	567	-5.259	22.966	2.318	1.00	48.66	O
ATOM	1891	C	GLU	A	567	-5.848	18.127	3.440	1.00	27.96	C
ATOM	1892	O	GLU	A	567	-6.553	17.189	3.829	1.00	27.68	O
ATOM	1893	N	LEU	A	568	-4.615	17.963	2.976	1.00	24.93	N
ATOM	1894	CA	LEU	A	568	-4.002	16.658	2.906	1.00	28.04	C
ATOM	1895	CB	LEU	A	568	-2.727	16.761	2.076	1.00	31.66	C
ATOM	1896	CG	LEU	A	568	-2.401	15.622	1.133	1.00	34.34	C
ATOM	1897	CD1	LEU	A	568	-3.680	15.015	0.564	1.00	38.44	C
ATOM	1898	CD2	LEU	A	568	-1.519	16.182	0.013	1.00	25.83	C
ATOM	1899	C	LEU	A	568	-3.700	16.146	4.307	1.00	30.03	C
ATOM	1900	O	LEU	A	568	-3.906	14.963	4.591	1.00	26.77	O
ATOM	1901	N	TYR	A	569	-3.199	17.016	5.187	1.00	24.67	N
ATOM	1902	CA	TYR	A	569	-2.947	16.534	6.538	1.00	22.81	C
ATOM	1903	CB	TYR	A	569	-2.176	17.572	7.375	1.00	21.70	C
ATOM	1904	CG	TYR	A	569	-1.824	17.040	8.753	1.00	21.77	C
ATOM	1905	CD1	TYR	A	569	-0.996	15.920	8.895	1.00	23.70	C
ATOM	1906	CE1	TYR	A	569	-0.720	15.375	10.158	1.00	23.93	C
ATOM	1907	CD2	TYR	A	569	-2.371	17.614	9.912	1.00	26.51	C
ATOM	1908	CE2	TYR	A	569	-2.107	17.074	11.184	1.00	29.40	C
ATOM	1909	CZ	TYR	A	569	-1.288	15.960	11.297	1.00	28.24	C
ATOM	1910	OH	TYR	A	569	-1.060	15.430	12.544	1.00	25.64	O
ATOM	1911	C	TYR	A	569	-4.270	16.175	7.234	1.00	23.78	C
ATOM	1912	O	TYR	A	569	-4.326	15.199	7.999	1.00	22.51	O
ATOM	1913	N	ALA	A	570	-5.339	16.936	6.983	1.00	23.61	N
ATOM	1914	CA	ALA	A	570	-6.621	16.634	7.632	1.00	26.10	C
ATOM	1915	CB	ALA	A	570	-7.710	17.646	7.202	1.00	26.46	C
ATOM	1916	C	ALA	A	570	-7.091	15.225	7.308	1.00	24.49	C
ATOM	1917	O	ALA	A	570	-7.666	14.532	8.162	1.00	24.77	O
ATOM	1918	N	LEU	A	571	-6.855	14.806	6.074	1.00	23.99	N
ATOM	1919	CA	LEU	A	571	-7.263	13.499	5.589	1.00	21.89	C
ATOM	1920	CB	LEU	A	571	-7.092	13.432	4.065	1.00	25.02	C
ATOM	1921	CG	LEU	A	571	-7.346	12.049	3.472	1.00	23.70	C
ATOM	1922	CD1	LEU	A	571	-8.724	11.529	3.891	1.00	26.43	C
ATOM	1923	CD2	LEU	A	571	-7.236	12.135	1.953	1.00	26.11	C
ATOM	1924	C	LEU	A	571	-6.406	12.422	6.245	1.00	20.20	C
ATOM	1925	O	LEU	A	571	-6.895	11.428	6.757	1.00	21.42	O
ATOM	1926	N	MET	A	572	-5.105	12.652	6.205	1.00	21.26	N
ATOM	1927	CA	MET	A	572	-4.141	11.758	6.808	1.00	24.72	C
ATOM	1928	CB	MET	A	572	-2.771	12.434	6.700	1.00	30.40	C
ATOM	1929	CG	MET	A	572	-1.685	11.742	7.418	1.00	32.31	C
ATOM	1930	SD	MET	A	572	-0.160	12.660	7.265	1.00	26.55	S
ATOM	1931	CE	MET	A	572	-0.165	13.232	5.451	1.00	24.24	C
ATOM	1932	C	MET	A	572	-4.531	11.574	8.280	1.00	22.05	C
ATOM	1933	O	MET	A	572	-4.607	10.448	8.782	1.00	23.12	O

ATOM	1934	N	SER	A	573	-4.796	12.686	8.965	1.00	18.21	N
ATOM	1935	CA	SER	A	573	-5.158	12.630	10.390	1.00	21.72	C
ATOM	1936	CB	SER	A	573	-5.155	14.055	10.973	1.00	21.94	C
ATOM	1937	OG	SER	A	573	-5.574	14.093	12.330	1.00	26.24	O
ATOM	1938	C	SER	A	573	-6.498	11.920	10.625	1.00	26.16	C
ATOM	1939	O	SER	A	573	-6.660	11.195	11.599	1.00	21.94	O
ATOM	1940	N	ASP	A	574	-7.471	12.122	9.749	1.00	21.50	N
ATOM	1941	CA	ASP	A	574	-8.748	11.427	9.902	1.00	22.60	C
ATOM	1942	CB	ASP	A	574	-9.791	11.915	8.883	1.00	20.64	C
ATOM	1943	CG	ASP	A	574	-10.332	13.301	9.213	1.00	23.27	C
ATOM	1944	OD1	ASP	A	574	-10.160	13.772	10.360	1.00	22.69	O
ATOM	1945	OD2	ASP	A	574	-10.966	13.888	8.314	1.00	26.93	O
ATOM	1946	C	ASP	A	574	-8.577	9.902	9.750	1.00	22.37	C
ATOM	1947	O	ASP	A	574	-9.359	9.141	10.333	1.00	23.59	O
ATOM	1948	N	CYS	A	575	-7.583	9.453	8.976	1.00	18.61	N
ATOM	1949	CA	CYS	A	575	-7.339	8.014	8.820	1.00	17.32	C
ATOM	1950	CB	CYS	A	575	-6.264	7.728	7.762	1.00	20.93	C
ATOM	1951	SG	CYS	A	575	-6.765	8.124	6.035	1.00	23.46	S
ATOM	1952	C	CYS	A	575	-6.855	7.431	10.156	1.00	21.12	C
ATOM	1953	O	CYS	A	575	-6.857	6.215	10.343	1.00	19.67	O
ATOM	1954	N	TRP	A	576	-6.423	8.322	11.047	1.00	19.86	N
ATOM	1955	CA	TRP	A	576	-5.934	7.931	12.370	1.00	21.52	C
ATOM	1956	CB	TRP	A	576	-4.611	8.626	12.709	1.00	20.08	C
ATOM	1957	CG	TRP	A	576	-3.521	8.406	11.707	1.00	19.69	C
ATOM	1958	CD2	TRP	A	576	-2.500	9.333	11.360	1.00	16.53	C
ATOM	1959	CE2	TRP	A	576	-1.694	8.716	10.367	1.00	18.10	C
ATOM	1960	CE3	TRP	A	576	-2.180	10.634	11.796	1.00	17.50	C
ATOM	1961	CD1	TRP	A	576	-3.312	7.284	10.950	1.00	20.54	C
ATOM	1962	NE1	TRP	A	576	-2.207	7.464	10.137	1.00	18.64	N
ATOM	1963	CZ2	TRP	A	576	-0.584	9.357	9.790	1.00	20.52	C
ATOM	1964	CZ3	TRP	A	576	-1.064	11.282	11.231	1.00	19.63	C
ATOM	1965	CH2	TRP	A	576	-0.280	10.638	10.231	1.00	18.57	C
ATOM	1966	C	TRP	A	576	-6.914	8.185	13.520	1.00	21.81	C
ATOM	1967	O	TRP	A	576	-6.487	8.424	14.664	1.00	21.51	O
ATOM	1968	N	ILE	A	577	-8.211	8.166	13.200	1.00	19.65	N
ATOM	1969	CA	ILE	A	577	-9.247	8.325	14.224	1.00	20.80	C
ATOM	1970	CB	ILE	A	577	-10.637	8.526	13.566	1.00	22.18	C
ATOM	1971	CG2	ILE	A	577	-11.783	8.179	14.574	1.00	20.80	C
ATOM	1972	CG1	ILE	A	577	-10.749	9.997	13.091	1.00	27.26	C
ATOM	1973	CD1	ILE	A	577	-11.997	10.298	12.254	1.00	29.41	C
ATOM	1974	C	ILE	A	577	-9.194	7.014	15.029	1.00	18.87	C
ATOM	1975	O	ILE	A	577	-9.204	5.927	14.455	1.00	21.86	O
ATOM	1976	N	TYR	A	578	-9.099	7.143	16.349	1.00	20.88	N
ATOM	1977	CA	TYR	A	578	-8.958	5.973	17.210	1.00	25.32	C
ATOM	1978	CB	TYR	A	578	-8.815	6.429	18.672	1.00	23.94	C
ATOM	1979	CG	TYR	A	578	-8.350	5.327	19.619	1.00	26.11	C
ATOM	1980	CD1	TYR	A	578	-7.000	5.188	19.946	1.00	31.42	C
ATOM	1981	CE1	TYR	A	578	-6.561	4.141	20.787	1.00	32.15	C
ATOM	1982	CD2	TYR	A	578	-9.256	4.401	20.158	1.00	33.33	C
ATOM	1983	CE2	TYR	A	578	-8.820	3.354	20.991	1.00	33.06	C
ATOM	1984	CZ	TYR	A	578	-7.468	3.232	21.295	1.00	31.77	C
ATOM	1985	OH	TYR	A	578	-7.016	2.178	22.088	1.00	33.01	O
ATOM	1986	C	TYR	A	578	-10.080	4.947	17.108	1.00	27.02	C
ATOM	1987	O	TYR	A	578	-9.819	3.750	16.903	1.00	22.11	O
ATOM	1988	N	LYS	A	579	-11.313	5.418	17.310	1.00	24.58	N
ATOM	1989	CA	LYS	A	579	-12.500	4.583	17.290	1.00	27.83	C
ATOM	1990	CB	LYS	A	579	-13.727	5.372	17.776	1.00	29.76	C
ATOM	1991	CG	LYS	A	579	-13.639	5.869	19.229	1.00	39.10	C
ATOM	1992	CD	LYS	A	579	-14.979	6.478	19.709	1.00	42.19	C
ATOM	1993	CE	LYS	A	579	-14.918	6.879	21.192	1.00	50.93	C
ATOM	1994	NZ	LYS	A	579	-16.124	7.694	21.593	1.00	50.31	N
ATOM	1995	C	LYS	A	579	-12.774	4.050	15.904	1.00	29.39	C
ATOM	1996	O	LYS	A	579	-12.998	4.803	14.976	1.00	27.65	O
ATOM	1997	N	TRP	A	580	-12.772	2.729	15.802	1.00	26.39	N
ATOM	1998	CA	TRP	A	580	-13.012	2.038	14.544	1.00	31.72	C
ATOM	1999	CB	TRP	A	580	-13.087	0.542	14.847	1.00	33.80	C
ATOM	2000	CG	TRP	A	580	-13.287	-0.297	13.670	1.00	36.87	C
ATOM	2001	CD2	TRP	A	580	-14.500	-0.948	13.288	1.00	37.12	C

ATOM	2002	CE2	TRP	A	580	-14.230	-1.666	12.097	1.00	42.38	C
ATOM	2003	CE3	TRP	A	580	-15.792	-0.998	13.835	1.00	43.97	C
ATOM	2004	CD1	TRP	A	580	-12.355	-0.624	12.728	1.00	41.08	C
ATOM	2005	NE1	TRP	A	580	-12.915	-1.452	11.777	1.00	37.64	N
ATOM	2006	CZ2	TRP	A	580	-15.205	-2.428	11.440	1.00	40.07	C
ATOM	2007	CZ3	TRP	A	580	-16.766	-1.757	13.182	1.00	45.16	C
ATOM	2008	CH2	TRP	A	580	-16.464	-2.462	11.996	1.00	48.53	C
ATOM	2009	C	TRP	A	580	-14.297	2.492	13.847	1.00	32.01	C
ATOM	2010	O	TRP	A	580	-14.300	2.806	12.651	1.00	29.01	O
ATOM	2011	N	GLU	A	581	-15.395	2.528	14.590	1.00	26.90	N
ATOM	2012	CA	GLU	A	581	-16.673	2.930	14.006	1.00	31.38	C
ATOM	2013	CB	GLU	A	581	-17.785	2.761	15.043	1.00	42.49	C
ATOM	2014	CG	GLU	A	581	-17.518	1.642	16.043	1.00	44.23	C
ATOM	2015	CD	GLU	A	581	-16.725	2.134	17.243	1.00	54.00	C
ATOM	2016	OE1	GLU	A	581	-17.263	2.985	17.997	1.00	62.87	O
ATOM	2017	OE2	GLU	A	581	-15.576	1.686	17.440	1.00	44.35	O
ATOM	2018	C	GLU	A	581	-16.703	4.365	13.461	1.00	31.42	C
ATOM	2019	O	GLU	A	581	-17.501	4.671	12.585	1.00	32.84	O
ATOM	2020	N	ASP	A	582	-15.824	5.232	13.963	1.00	29.31	N
ATOM	2021	CA	ASP	A	582	-15.779	6.631	13.543	1.00	26.27	C
ATOM	2022	CB	ASP	A	582	-15.502	7.525	14.759	1.00	30.65	C
ATOM	2023	CG	ASP	A	582	-16.611	7.449	15.799	1.00	38.03	C
ATOM	2024	OD1	ASP	A	582	-17.741	7.089	15.416	1.00	34.32	O
ATOM	2025	OD2	ASP	A	582	-16.357	7.744	16.989	1.00	35.77	O
ATOM	2026	C	ASP	A	582	-14.741	6.955	12.458	1.00	28.97	C
ATOM	2027	O	ASP	A	582	-14.682	8.086	11.957	1.00	25.58	O
ATOM	2028	N	ARG	A	583	-13.926	5.970	12.107	1.00	26.36	N
ATOM	2029	CA	ARG	A	583	-12.883	6.195	11.108	1.00	26.57	C
ATOM	2030	CB	ARG	A	583	-11.756	5.153	11.313	1.00	24.45	C
ATOM	2031	CG	ARG	A	583	-10.396	5.437	10.597	1.00	21.69	C
ATOM	2032	CD	ARG	A	583	-9.414	4.259	10.869	1.00	18.39	C
ATOM	2033	NE	ARG	A	583	-9.289	4.015	12.315	1.00	17.34	N
ATOM	2034	CZ	ARG	A	583	-9.081	2.825	12.866	1.00	21.68	C
ATOM	2035	NH1	ARG	A	583	-8.963	1.744	12.113	1.00	18.82	N
ATOM	2036	NH2	ARG	A	583	-9.029	2.717	14.200	1.00	22.38	N
ATOM	2037	C	ARG	A	583	-13.525	6.070	9.720	1.00	24.67	C
ATOM	2038	O	ARG	A	583	-14.382	5.223	9.485	1.00	25.78	O
ATOM	2039	N	PRO	A	584	-13.109	6.916	8.769	1.00	23.39	N
ATOM	2040	CD	PRO	A	584	-12.146	8.027	8.893	1.00	25.28	C
ATOM	2041	CA	PRO	A	584	-13.667	6.869	7.407	1.00	25.72	C
ATOM	2042	CB	PRO	A	584	-13.073	8.097	6.736	1.00	26.27	C
ATOM	2043	CG	PRO	A	584	-11.760	8.276	7.437	1.00	22.96	C
ATOM	2044	C	PRO	A	584	-13.318	5.609	6.620	1.00	26.41	C
ATOM	2045	O	PRO	A	584	-12.329	4.940	6.930	1.00	23.65	O
ATOM	2046	N	ASP	A	585	-14.142	5.313	5.610	1.00	20.71	N
ATOM	2047	CA	ASP	A	585	-13.920	4.182	4.714	1.00	20.68	C
ATOM	2048	CB	ASP	A	585	-15.258	3.578	4.236	1.00	31.23	C
ATOM	2049	CG	ASP	A	585	-16.100	3.042	5.380	1.00	41.40	C
ATOM	2050	OD1	ASP	A	585	-15.581	2.249	6.197	1.00	48.33	O
ATOM	2051	OD2	ASP	A	585	-17.295	3.419	5.453	1.00	55.79	O
ATOM	2052	C	ASP	A	585	-13.183	4.695	3.471	1.00	19.99	C
ATOM	2053	O	ASP	A	585	-13.097	5.907	3.256	1.00	24.11	O
ATOM	2054	N	PHE	A	586	-12.692	3.777	2.636	1.00	21.55	N
ATOM	2055	CA	PHE	A	586	-11.960	4.193	1.439	1.00	25.44	C
ATOM	2056	CB	PHE	A	586	-11.231	3.013	0.780	1.00	23.78	C
ATOM	2057	CG	PHE	A	586	-9.909	2.689	1.445	1.00	21.80	C
ATOM	2058	CD1	PHE	A	586	-8.837	3.578	1.392	1.00	26.67	C
ATOM	2059	CD2	PHE	A	586	-9.754	1.480	2.146	1.00	26.93	C
ATOM	2060	CE1	PHE	A	586	-7.606	3.261	2.026	1.00	19.00	C
ATOM	2061	CE2	PHE	A	586	-8.546	1.175	2.767	1.00	22.77	C
ATOM	2062	CZ	PHE	A	586	-7.482	2.056	2.701	1.00	20.88	C
ATOM	2063	C	PHE	A	586	-12.863	4.894	0.430	1.00	25.78	C
ATOM	2064	O	PHE	A	586	-12.399	5.669	-0.358	1.00	22.13	O
ATOM	2065	N	LEU	A	587	-14.168	4.628	0.487	1.00	27.35	N
ATOM	2066	CA	LEU	A	587	-15.082	5.342	-0.410	1.00	27.54	C
ATOM	2067	CB	LEU	A	587	-16.525	4.916	-0.107	1.00	33.35	C
ATOM	2068	CG	LEU	A	587	-17.649	5.418	-1.010	1.00	40.50	C
ATOM	2069	CD1	LEU	A	587	-17.775	6.902	-0.854	1.00	43.82	C

ATOM	2070	CD2	LEU	A	587	-17.358	5.069	-2.455	1.00	41.16	C
ATOM	2071	C	LEU	A	587	-14.879	6.856	-0.178	1.00	21.74	C
ATOM	2072	O	LEU	A	587	-14.638	7.596	-1.137	1.00	29.01	O
ATOM	2073	N	THR	A	588	-14.923	7.322	1.077	1.00	21.57	N
ATOM	2074	CA	THR	A	588	-14.718	8.743	1.326	1.00	25.49	C
ATOM	2075	CB	THR	A	588	-15.271	9.205	2.705	1.00	35.32	C
ATOM	2076	OG1	THR	A	588	-14.462	8.694	3.759	1.00	46.78	O
ATOM	2077	CG2	THR	A	588	-16.687	8.707	2.879	1.00	33.61	C
ATOM	2078	C	THR	A	588	-13.257	9.153	1.212	1.00	28.40	C
ATOM	2079	O	THR	A	588	-12.964	10.229	0.705	1.00	26.45	O
ATOM	2080	N	VAL	A	589	-12.341	8.293	1.670	1.00	22.28	N
ATOM	2081	CA	VAL	A	589	-10.927	8.646	1.549	1.00	19.94	C
ATOM	2082	CB	VAL	A	589	-10.021	7.525	2.161	1.00	27.25	C
ATOM	2083	CG1	VAL	A	589	-8.539	7.770	1.790	1.00	22.69	C
ATOM	2084	CG2	VAL	A	589	-10.180	7.525	3.673	1.00	24.26	C
ATOM	2085	C	VAL	A	589	-10.502	8.911	0.102	1.00	20.96	C
ATOM	2086	O	VAL	A	589	-9.788	9.888	-0.178	1.00	21.66	O
ATOM	2087	N	GLU	A	590	-10.932	8.047	-0.818	1.00	23.06	N
ATOM	2088	CA	GLU	A	590	-10.583	8.205	-2.227	1.00	22.93	C
ATOM	2089	CB	GLU	A	590	-11.130	7.022	-3.049	1.00	24.91	C
ATOM	2090	CG	GLU	A	590	-10.775	7.021	-4.559	1.00	27.15	C
ATOM	2091	CD	GLU	A	590	-11.603	8.014	-5.414	1.00	31.97	C
ATOM	2092	OE1	GLU	A	590	-12.804	8.214	-5.130	1.00	31.00	O
ATOM	2093	OE2	GLU	A	590	-11.056	8.562	-6.399	1.00	29.57	O
ATOM	2094	C	GLU	A	590	-11.137	9.531	-2.784	1.00	25.86	C
ATOM	2095	O	GLU	A	590	-10.466	10.218	-3.552	1.00	21.69	O
ATOM	2096	N	GLN	A	591	-12.362	9.875	-2.394	1.00	24.00	N
ATOM	2097	CA	GLN	A	591	-12.972	11.131	-2.856	1.00	27.84	C
ATOM	2098	CB	GLN	A	591	-14.426	11.197	-2.398	1.00	29.39	C
ATOM	2099	CG	GLN	A	591	-15.298	10.136	-2.993	1.00	32.75	C
ATOM	2100	CD	GLN	A	591	-16.754	10.334	-2.629	1.00	38.78	C
ATOM	2101	OE1	GLN	A	591	-17.078	11.132	-1.745	1.00	43.77	O
ATOM	2102	NE2	GLN	A	591	-17.636	9.614	-3.302	1.00	44.60	N
ATOM	2103	C	GLN	A	591	-12.240	12.361	-2.354	1.00	28.08	C
ATOM	2104	O	GLN	A	591	-12.023	13.332	-3.097	1.00	27.52	O
ATOM	2105	N	ARG	A	592	-11.851	12.345	-1.084	1.00	24.43	N
ATOM	2106	CA	ARG	A	592	-11.138	13.471	-0.520	1.00	25.06	C
ATOM	2107	CB	ARG	A	592	-11.060	13.338	1.004	1.00	25.79	C
ATOM	2108	CG	ARG	A	592	-12.433	13.494	1.649	1.00	28.74	C
ATOM	2109	CD	ARG	A	592	-12.418	13.215	3.127	1.00	31.24	C
ATOM	2110	NE	ARG	A	592	-11.576	14.162	3.844	1.00	25.60	N
ATOM	2111	CZ	ARG	A	592	-11.336	14.096	5.146	1.00	25.97	C
ATOM	2112	NH1	ARG	A	592	-11.883	13.123	5.859	1.00	27.29	N
ATOM	2113	NH2	ARG	A	592	-10.551	14.996	5.720	1.00	28.63	N
ATOM	2114	C	ARG	A	592	-9.750	13.563	-1.117	1.00	25.17	C
ATOM	2115	O	ARG	A	592	-9.235	14.667	-1.360	1.00	26.90	O
ATOM	2116	N	MET	A	593	-9.138	12.409	-1.368	1.00	23.69	N
ATOM	2117	CA	MET	A	593	-7.796	12.416	-1.931	1.00	28.31	C
ATOM	2118	CB	MET	A	593	-7.192	11.000	-1.892	1.00	23.46	C
ATOM	2119	CG	MET	A	593	-5.743	10.934	-2.292	1.00	23.72	C
ATOM	2120	SD	MET	A	593	-4.646	11.896	-1.177	1.00	28.98	S
ATOM	2121	CE	MET	A	593	-3.866	12.944	-2.359	1.00	26.58	C
ATOM	2122	C	MET	A	593	-7.862	12.937	-3.372	1.00	26.14	C
ATOM	2123	O	MET	A	593	-6.998	13.697	-3.802	1.00	28.83	O
ATOM	2124	N	ARG	A	594	-8.877	12.519	-4.117	1.00	23.87	N
ATOM	2125	CA	ARG	A	594	-9.023	12.958	-5.498	1.00	24.90	C
ATOM	2126	CB	ARG	A	594	-10.275	12.328	-6.106	1.00	21.24	C
ATOM	2127	CG	ARG	A	594	-10.482	12.694	-7.596	1.00	25.80	C
ATOM	2128	CD	ARG	A	594	-11.817	12.169	-8.118	1.00	36.37	C
ATOM	2129	NE	ARG	A	594	-11.832	10.715	-8.236	1.00	43.01	N
ATOM	2130	CZ	ARG	A	594	-11.353	10.041	-9.281	1.00	44.29	C
ATOM	2131	NH1	ARG	A	594	-10.823	10.690	-10.313	1.00	45.97	N
ATOM	2132	NH2	ARG	A	594	-11.387	8.716	-9.289	1.00	38.74	N
ATOM	2133	C	ARG	A	594	-9.116	14.494	-5.542	1.00	28.27	C
ATOM	2134	O	ARG	A	594	-8.465	15.150	-6.362	1.00	30.97	O
ATOM	2135	N	ALA	A	595	-9.911	15.050	-4.637	1.00	30.31	N
ATOM	2136	CA	ALA	A	595	-10.118	16.495	-4.530	1.00	34.21	C
ATOM	2137	CB	ALA	A	595	-11.224	16.787	-3.496	1.00	32.96	C

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ATOM   2138  C   ALA A 595      -8.834  17.234  -4.161  1.00 36.64           C
ATOM   2139  O   ALA A 595      -8.550  18.300  -4.705  1.00 34.21           O
ATOM   2140  N   CYS A 596      -8.057  16.664  -3.237  1.00 31.92           N
ATOM   2141  CA  CYS A 596      -6.803  17.277  -2.826  1.00 33.56           C
ATOM   2142  CB  CYS A 596      -6.169  16.505  -1.655  1.00 31.86           C
ATOM   2143  SG  CYS A 596      -7.012  16.710  -0.074  1.00 40.76           S
ATOM   2144  C   CYS A 596      -5.830  17.280  -3.990  1.00 32.72           C
ATOM   2145  O   CYS A 596      -5.155  18.279  -4.245  1.00 31.91           O
ATOM   2146  N   TYR A 597      -5.747  16.150  -4.686  1.00 28.25           N
ATOM   2147  CA  TYR A 597      -4.832  16.036  -5.814  1.00 30.48           C
ATOM   2148  CB  TYR A 597      -4.881  14.615  -6.389  1.00 31.14           C
ATOM   2149  CG  TYR A 597      -4.225  14.464  -7.742  1.00 31.11           C
ATOM   2150  CD1 TYR A 597      -2.963  15.000  -7.993  1.00 32.87           C
ATOM   2151  CE1 TYR A 597      -2.370  14.894  -9.259  1.00 37.85           C
ATOM   2152  CD2 TYR A 597      -4.877  13.806  -8.780  1.00 34.93           C
ATOM   2153  CE2 TYR A 597      -4.298  13.687 -10.047  1.00 41.03           C
ATOM   2154  CZ  TYR A 597      -3.048  14.240 -10.281  1.00 39.13           C
ATOM   2155  OH  TYR A 597      -2.505  14.165 -11.543  1.00 39.42           O
ATOM   2156  C   TYR A 597      -5.168  17.049  -6.907  1.00 34.57           C
ATOM   2157  O   TYR A 597      -4.275  17.751  -7.421  1.00 33.33           O
ATOM   2158  N   TYR A 598      -6.446  17.106  -7.261  1.00 30.49           N
ATOM   2159  CA  TYR A 598      -6.921  18.019  -8.298  1.00 40.96           C
ATOM   2160  CB  TYR A 598      -8.427  17.833  -8.532  1.00 38.84           C
ATOM   2161  CG  TYR A 598      -8.800  16.590  -9.316  1.00 41.02           C
ATOM   2162  CD1 TYR A 598     -10.130  16.335  -9.659  1.00 49.62           C
ATOM   2163  CE1 TYR A 598     -10.490  15.170 -10.353  1.00 49.11           C
ATOM   2164  CD2 TYR A 598      -7.838  15.651  -9.691  1.00 46.14           C
ATOM   2165  CE2 TYR A 598      -8.182  14.489 -10.377  1.00 45.32           C
ATOM   2166  CZ  TYR A 598      -9.511  14.252 -10.703  1.00 50.82           C
ATOM   2167  OH  TYR A 598      -9.857  13.082 -11.342  1.00 48.64           O
ATOM   2168  C   TYR A 598      -6.630  19.453  -7.903  1.00 44.26           C
ATOM   2169  O   TYR A 598      -6.255  20.275  -8.744  1.00 50.25           O
ATOM   2170  N   SER A 599      -6.790  19.759  -6.623  1.00 36.48           N
ATOM   2171  CA  SER A 599      -6.525  21.095  -6.132  1.00 42.68           C
ATOM   2172  CB  SER A 599      -6.935  21.185  -4.670  1.00 43.70           C
ATOM   2173  OG  SER A 599      -6.732  22.487  -4.171  1.00 57.23           O
ATOM   2174  C   SER A 599      -5.035  21.427  -6.295  1.00 46.61           C
ATOM   2175  O   SER A 599      -4.663  22.541  -6.686  1.00 38.28           O
ATOM   2176  N   LEU A 600      -4.176  20.459  -6.006  1.00 35.37           N
ATOM   2177  CA  LEU A 600      -2.740  20.681  -6.137  1.00 43.98           C
ATOM   2178  CB  LEU A 600      -1.955  19.613  -5.372  1.00 36.49           C
ATOM   2179  CG  LEU A 600      -2.119  19.658  -3.850  1.00 42.50           C
ATOM   2180  CD1 LEU A 600      -1.522  18.409  -3.229  1.00 35.50           C
ATOM   2181  CD2 LEU A 600      -1.449  20.896  -3.293  1.00 45.68           C
ATOM   2182  C   LEU A 600      -2.301  20.674  -7.587  1.00 41.54           C
ATOM   2183  O   LEU A 600      -1.381  21.406  -7.965  1.00 46.25           O
ATOM   2184  N   ALA A 601      -2.963  19.850  -8.393  1.00 38.74           N
ATOM   2185  CA  ALA A 601      -2.648  19.698  -9.811  1.00 47.05           C
ATOM   2186  CB  ALA A 601      -3.470  18.564 -10.404  1.00 45.68           C
ATOM   2187  C   ALA A 601      -2.912  20.997 -10.569  1.00 52.87           C
ATOM   2188  O   ALA A 601      -2.239  21.306 -11.556  1.00 53.37           O
ATOM   2189  N   SER A 602      -3.899  21.748 -10.094  1.00 51.50           N
ATOM   2190  CA  SER A 602      -4.266  23.024 -10.691  1.00 57.64           C
ATOM   2191  CB  SER A 602      -5.750  23.293 -10.458  1.00 57.42           C
ATOM   2192  OG  SER A 602      -6.542  22.301 -11.091  1.00 55.95           O
ATOM   2193  C   SER A 602      -3.428  24.130 -10.054  1.00 59.56           C
ATOM   2194  O   SER A 602      -3.790  25.302 -10.103  1.00 64.84           O
ATOM   2195  N   LYS A 603      -2.307  23.730  -9.459  1.00 63.84           N
ATOM   2196  CA  LYS A 603      -1.378  24.639  -8.792  1.00 65.05           C
ATOM   2197  CB  LYS A 603      -0.968  25.767  -9.747  1.00 65.01           C
ATOM   2198  CG  LYS A 603       0.509  26.120  -9.697  1.00 65.21           C
ATOM   2199  CD  LYS A 603       0.835  27.209 -10.706  1.00 65.84           C
ATOM   2200  CE  LYS A 603       2.334  27.480 -10.766  1.00 67.72           C
ATOM   2201  NZ  LYS A 603       2.656  28.634 -11.659  1.00 67.84           N
ATOM   2202  C   LYS A 603      -2.011  25.214  -7.519  1.00 65.66           C
ATOM   2203  O   LYS A 603      -1.435  25.016  -6.424  1.00 67.21           O
ATOM   2204  OXT LYS A 603      -3.085  25.847  -7.626  1.00 69.14           O
TER       1      LYS A 603
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ATOM	2205	CB	PHE	B	331	26.385	4.944	44.783	1.00	47.38	C
ATOM	2206	CG	PHE	B	331	26.386	4.527	43.338	1.00	47.76	C
ATOM	2207	CD1	PHE	B	331	27.574	4.465	42.621	1.00	52.74	C
ATOM	2208	CD2	PHE	B	331	25.201	4.218	42.689	1.00	47.87	C
ATOM	2209	CE1	PHE	B	331	27.582	4.104	41.283	1.00	48.41	C
ATOM	2210	CE2	PHE	B	331	25.196	3.855	41.347	1.00	52.09	C
ATOM	2211	CZ	PHE	B	331	26.387	3.797	40.643	1.00	50.05	C
ATOM	2212	C	PHE	B	331	26.230	6.878	46.363	1.00	45.38	C
ATOM	2213	O	PHE	B	331	27.005	6.988	47.313	1.00	49.66	O
ATOM	2214	N	PHE	B	331	28.209	6.632	44.860	1.00	48.36	N
ATOM	2215	CA	PHE	B	331	26.733	6.417	44.999	1.00	44.38	C
ATOM	2216	N	LEU	B	332	24.933	7.156	46.441	1.00	39.16	N
ATOM	2217	CA	LEU	B	332	24.306	7.623	47.678	1.00	40.71	C
ATOM	2218	CB	LEU	B	332	23.601	8.967	47.426	1.00	40.95	C
ATOM	2219	CG	LEU	B	332	24.412	10.129	46.828	1.00	42.67	C
ATOM	2220	CD1	LEU	B	332	23.451	11.230	46.342	1.00	38.80	C
ATOM	2221	CD2	LEU	B	332	25.394	10.684	47.864	1.00	39.78	C
ATOM	2222	C	LEU	B	332	23.276	6.592	48.138	1.00	42.07	C
ATOM	2223	O	LEU	B	332	22.808	5.781	47.347	1.00	39.83	O
ATOM	2224	N	LYS	B	333	22.929	6.621	49.423	1.00	42.54	N
ATOM	2225	CA	LYS	B	333	21.927	5.699	49.947	1.00	44.61	C
ATOM	2226	CB	LYS	B	333	22.050	5.571	51.467	1.00	46.09	C
ATOM	2227	CG	LYS	B	333	23.341	4.930	51.902	1.00	50.67	C
ATOM	2228	CD	LYS	B	333	23.230	4.443	53.337	1.00	58.35	C
ATOM	2229	CE	LYS	B	333	24.498	3.707	53.764	1.00	59.84	C
ATOM	2230	NZ	LYS	B	333	24.351	3.125	55.132	1.00	62.41	N
ATOM	2231	C	LYS	B	333	20.542	6.206	49.605	1.00	41.31	C
ATOM	2232	O	LYS	B	333	20.214	7.357	49.888	1.00	39.53	O
ATOM	2233	N	ARG	B	334	19.729	5.332	49.021	1.00	36.95	N
ATOM	2234	CA	ARG	B	334	18.375	5.682	48.628	1.00	43.46	C
ATOM	2235	CB	ARG	B	334	17.707	4.487	47.944	1.00	44.85	C
ATOM	2236	CG	ARG	B	334	16.275	4.735	47.485	1.00	43.32	C
ATOM	2237	CD	ARG	B	334	16.238	5.676	46.299	1.00	38.79	C
ATOM	2238	NE	ARG	B	334	14.873	5.974	45.879	1.00	37.97	N
ATOM	2239	CZ	ARG	B	334	14.074	6.819	46.509	1.00	38.57	C
ATOM	2240	NH1	ARG	B	334	14.505	7.457	47.595	1.00	36.94	N
ATOM	2241	NH2	ARG	B	334	12.846	7.038	46.054	1.00	42.39	N
ATOM	2242	C	ARG	B	334	17.547	6.103	49.839	1.00	45.57	C
ATOM	2243	O	ARG	B	334	16.571	6.845	49.712	1.00	41.28	O
ATOM	2244	N	ASP	B	335	17.960	5.619	51.010	1.00	46.31	N
ATOM	2245	CA	ASP	B	335	17.274	5.898	52.272	1.00	45.57	C
ATOM	2246	CB	ASP	B	335	17.823	4.969	53.354	1.00	51.22	C
ATOM	2247	CG	ASP	B	335	17.911	3.533	52.887	1.00	54.98	C
ATOM	2248	OD1	ASP	B	335	16.856	2.869	52.816	1.00	60.53	O
ATOM	2249	OD2	ASP	B	335	19.032	3.074	52.567	1.00	62.94	O
ATOM	2250	C	ASP	B	335	17.439	7.338	52.719	1.00	42.46	C
ATOM	2251	O	ASP	B	335	16.647	7.840	53.525	1.00	36.68	O
ATOM	2252	N	ASN	B	336	18.471	8.010	52.219	1.00	29.28	N
ATOM	2253	CA	ASN	B	336	18.713	9.383	52.603	1.00	31.89	C
ATOM	2254	CB	ASN	B	336	20.211	9.667	52.652	1.00	33.88	C
ATOM	2255	CG	ASN	B	336	20.904	8.875	53.734	1.00	49.73	C
ATOM	2256	OD1	ASN	B	336	20.356	8.676	54.822	1.00	46.67	O
ATOM	2257	ND2	ASN	B	336	22.124	8.437	53.452	1.00	47.83	N
ATOM	2258	C	ASN	B	336	18.054	10.366	51.655	1.00	27.35	C
ATOM	2259	O	ASN	B	336	18.188	11.571	51.819	1.00	28.55	O
ATOM	2260	N	LEU	B	337	17.341	9.834	50.679	1.00	31.14	N
ATOM	2261	CA	LEU	B	337	16.687	10.667	49.677	1.00	34.02	C
ATOM	2262	CB	LEU	B	337	17.174	10.263	48.277	1.00	30.37	C
ATOM	2263	CG	LEU	B	337	16.623	11.013	47.049	1.00	29.39	C
ATOM	2264	CD1	LEU	B	337	17.255	12.379	46.971	1.00	29.26	C
ATOM	2265	CD2	LEU	B	337	16.949	10.246	45.775	1.00	35.80	C
ATOM	2266	C	LEU	B	337	15.163	10.583	49.728	1.00	29.91	C
ATOM	2267	O	LEU	B	337	14.581	9.510	49.799	1.00	30.87	O
ATOM	2268	N	LEU	B	338	14.516	11.733	49.674	1.00	26.54	N
ATOM	2269	CA	LEU	B	338	13.060	11.780	49.667	1.00	26.34	C
ATOM	2270	CB	LEU	B	338	12.534	12.524	50.910	1.00	27.85	C
ATOM	2271	CG	LEU	B	338	10.999	12.521	51.023	1.00	29.64	C
ATOM	2272	CD1	LEU	B	338	10.508	11.097	51.215	1.00	34.52	C

ATOM	2273	CD2	LEU	B	338	10.550	13.388	52.184	1.00	29.92	C
ATOM	2274	C	LEU	B	338	12.693	12.562	48.397	1.00	29.11	C
ATOM	2275	O	LEU	B	338	12.941	13.762	48.321	1.00	29.08	O
ATOM	2276	N	ILE	B	339	12.145	11.868	47.402	1.00	29.57	N
ATOM	2277	CA	ILE	B	339	11.785	12.534	46.150	1.00	28.48	C
ATOM	2278	CB	ILE	B	339	11.902	11.564	44.950	1.00	32.66	C
ATOM	2279	CG2	ILE	B	339	11.633	12.331	43.627	1.00	32.51	C
ATOM	2280	CG1	ILE	B	339	13.286	10.909	44.961	1.00	32.18	C
ATOM	2281	CD1	ILE	B	339	13.495	9.849	43.902	1.00	41.01	C
ATOM	2282	C	ILE	B	339	10.366	13.062	46.208	1.00	31.19	C
ATOM	2283	O	ILE	B	339	9.431	12.309	46.466	1.00	33.54	O
ATOM	2284	N	ALA	B	340	10.208	14.358	45.965	1.00	28.66	N
ATOM	2285	CA	ALA	B	340	8.880	14.966	45.989	1.00	34.20	C
ATOM	2286	CB	ALA	B	340	8.990	16.462	46.265	1.00	32.40	C
ATOM	2287	C	ALA	B	340	8.152	14.717	44.667	1.00	36.35	C
ATOM	2288	O	ALA	B	340	8.775	14.336	43.663	1.00	35.42	O
ATOM	2289	N	ASP	B	341	6.836	14.907	44.674	1.00	33.98	N
ATOM	2290	CA	ASP	B	341	6.041	14.711	43.469	1.00	39.65	C
ATOM	2291	CB	ASP	B	341	4.631	14.226	43.840	1.00	45.61	C
ATOM	2292	CG	ASP	B	341	3.912	13.554	42.670	1.00	57.27	C
ATOM	2293	OD1	ASP	B	341	4.096	14.002	41.519	1.00	59.44	O
ATOM	2294	OD2	ASP	B	341	3.149	12.582	42.901	1.00	63.51	O
ATOM	2295	C	ASP	B	341	5.959	16.070	42.779	1.00	44.29	C
ATOM	2296	O	ASP	B	341	4.868	16.568	42.502	1.00	45.33	O
ATOM	2297	N	ILE	B	342	7.119	16.671	42.514	1.00	36.54	N
ATOM	2298	CA	ILE	B	342	7.202	17.981	41.879	1.00	36.97	C
ATOM	2299	CB	ILE	B	342	7.661	19.043	42.896	1.00	38.63	C
ATOM	2300	CG2	ILE	B	342	7.852	20.397	42.215	1.00	42.84	C
ATOM	2301	CG1	ILE	B	342	6.645	19.131	44.033	1.00	39.67	C
ATOM	2302	CD1	ILE	B	342	7.093	20.032	45.166	1.00	46.12	C
ATOM	2303	C	ILE	B	342	8.225	17.899	40.753	1.00	37.86	C
ATOM	2304	O	ILE	B	342	9.336	17.438	40.961	1.00	33.45	O
ATOM	2305	N	GLU	B	343	7.840	18.335	39.561	1.00	31.27	N
ATOM	2306	CA	GLU	B	343	8.736	18.281	38.415	1.00	35.65	C
ATOM	2307	CB	GLU	B	343	7.994	17.733	37.194	1.00	35.13	C
ATOM	2308	CG	GLU	B	343	8.842	17.680	35.940	1.00	40.36	C
ATOM	2309	CD	GLU	B	343	8.204	16.874	34.824	1.00	49.77	C
ATOM	2310	OE1	GLU	B	343	8.173	15.627	34.926	1.00	48.98	O
ATOM	2311	OE2	GLU	B	343	7.734	17.488	33.845	1.00	50.13	O
ATOM	2312	C	GLU	B	343	9.287	19.661	38.112	1.00	35.92	C
ATOM	2313	O	GLU	B	343	8.522	20.568	37.825	1.00	33.14	O
ATOM	2314	N	LEU	B	344	10.612	19.811	38.179	1.00	26.19	N
ATOM	2315	CA	LEU	B	344	11.245	21.100	37.907	1.00	26.71	C
ATOM	2316	CB	LEU	B	344	12.646	21.179	38.577	1.00	25.66	C
ATOM	2317	CG	LEU	B	344	12.593	21.025	40.097	1.00	30.64	C
ATOM	2318	CD1	LEU	B	344	14.017	20.874	40.644	1.00	27.22	C
ATOM	2319	CD2	LEU	B	344	11.877	22.223	40.737	1.00	33.34	C
ATOM	2320	C	LEU	B	344	11.373	21.299	36.404	1.00	25.27	C
ATOM	2321	O	LEU	B	344	11.313	22.428	35.912	1.00	30.00	O
ATOM	2322	N	GLY	B	345	11.576	20.206	35.672	1.00	24.88	N
ATOM	2323	CA	GLY	B	345	11.683	20.297	34.228	1.00	29.60	C
ATOM	2324	C	GLY	B	345	11.779	18.915	33.635	1.00	29.46	C
ATOM	2325	O	GLY	B	345	11.720	17.929	34.366	1.00	32.49	O
ATOM	2326	N	CYS	B	346	11.915	18.818	32.315	1.00	27.20	N
ATOM	2327	CA	CYS	B	346	12.057	17.510	31.688	1.00	32.81	C
ATOM	2328	CB	CYS	B	346	10.690	16.909	31.391	1.00	41.74	C
ATOM	2329	SG	CYS	B	346	9.815	17.890	30.185	1.00	44.47	S
ATOM	2330	C	CYS	B	346	12.843	17.626	30.391	1.00	38.59	C
ATOM	2331	O	CYS	B	346	13.184	18.728	29.963	1.00	36.63	O
ATOM	2332	N	GLY	B	347	13.120	16.478	29.785	1.00	36.78	N
ATOM	2333	CA	GLY	B	347	13.846	16.426	28.528	1.00	36.32	C
ATOM	2334	C	GLY	B	347	13.632	15.050	27.936	1.00	37.34	C
ATOM	2335	O	GLY	B	347	12.888	14.252	28.505	1.00	35.37	O
ATOM	2336	N	ASN	B	348	14.274	14.760	26.812	1.00	38.30	N
ATOM	2337	CA	ASN	B	348	14.143	13.451	26.180	1.00	41.78	C
ATOM	2338	CB	ASN	B	348	14.905	13.414	24.850	1.00	50.03	C
ATOM	2339	CG	ASN	B	348	14.269	14.284	23.799	1.00	55.15	C
ATOM	2340	OD1	ASN	B	348	13.105	14.090	23.440	1.00	59.57	O

ATOM	2341	ND2	ASN	B	348	15.028	15.256	23.289	1.00	59.33	N
ATOM	2342	C	ASN	B	348	14.670	12.334	27.077	1.00	39.62	C
ATOM	2343	O	ASN	B	348	14.281	11.183	26.930	1.00	38.79	O
ATOM	2344	N	PHE	B	349	15.565	12.683	28.002	1.00	34.25	N
ATOM	2345	CA	PHE	B	349	16.144	11.700	28.915	1.00	36.33	C
ATOM	2346	CB	PHE	B	349	17.408	12.277	29.580	1.00	38.59	C
ATOM	2347	CG	PHE	B	349	17.140	13.471	30.459	1.00	35.63	C
ATOM	2348	CD1	PHE	B	349	16.529	13.315	31.702	1.00	37.36	C
ATOM	2349	CD2	PHE	B	349	17.441	14.759	30.022	1.00	35.00	C
ATOM	2350	CE1	PHE	B	349	16.216	14.431	32.496	1.00	36.08	C
ATOM	2351	CE2	PHE	B	349	17.135	15.872	30.805	1.00	39.51	C
ATOM	2352	CZ	PHE	B	349	16.518	15.707	32.047	1.00	34.21	C
ATOM	2353	C	PHE	B	349	15.156	11.303	30.014	1.00	34.30	C
ATOM	2354	O	PHE	B	349	15.219	10.212	30.562	1.00	37.30	O
ATOM	2355	N	GLY	B	350	14.263	12.220	30.358	1.00	34.85	N
ATOM	2356	CA	GLY	B	350	13.316	11.949	31.422	1.00	32.42	C
ATOM	2357	C	GLY	B	350	12.919	13.235	32.096	1.00	33.80	C
ATOM	2358	O	GLY	B	350	12.575	14.204	31.433	1.00	38.01	O
ATOM	2359	N	SER	B	351	12.954	13.274	33.421	1.00	34.81	N
ATOM	2360	CA	SER	B	351	12.560	14.497	34.079	1.00	31.64	C
ATOM	2361	CB	SER	B	351	11.114	14.395	34.536	1.00	42.24	C
ATOM	2362	OG	SER	B	351	10.994	13.473	35.583	1.00	38.56	O
ATOM	2363	C	SER	B	351	13.461	14.859	35.246	1.00	24.48	C
ATOM	2364	O	SER	B	351	14.303	14.076	35.670	1.00	31.02	O
ATOM	2365	N	VAL	B	352	13.276	16.064	35.751	1.00	23.21	N
ATOM	2366	CA	VAL	B	352	14.069	16.551	36.869	1.00	25.51	C
ATOM	2367	CB	VAL	B	352	14.776	17.865	36.521	1.00	23.36	C
ATOM	2368	CG1	VAL	B	352	15.570	18.356	37.728	1.00	28.15	C
ATOM	2369	CG2	VAL	B	352	15.710	17.645	35.316	1.00	25.42	C
ATOM	2370	C	VAL	B	352	13.051	16.809	37.964	1.00	25.74	C
ATOM	2371	O	VAL	B	352	12.153	17.661	37.818	1.00	26.16	O
ATOM	2372	N	ARG	B	353	13.208	16.078	39.059	1.00	22.97	N
ATOM	2373	CA	ARG	B	353	12.299	16.161	40.194	1.00	23.75	C
ATOM	2374	CB	ARG	B	353	11.909	14.745	40.652	1.00	25.68	C
ATOM	2375	CG	ARG	B	353	11.121	13.891	39.655	1.00	41.51	C
ATOM	2376	CD	ARG	B	353	9.703	14.400	39.449	1.00	48.70	C
ATOM	2377	NE	ARG	B	353	8.746	13.308	39.273	1.00	58.71	N
ATOM	2378	CZ	ARG	B	353	8.258	12.560	40.263	1.00	59.20	C
ATOM	2379	NH1	ARG	B	353	8.627	12.776	41.519	1.00	53.03	N
ATOM	2380	NH2	ARG	B	353	7.404	11.579	39.992	1.00	59.16	N
ATOM	2381	C	ARG	B	353	12.924	16.882	41.366	1.00	29.40	C
ATOM	2382	O	ARG	B	353	14.147	16.866	41.554	1.00	30.85	O
ATOM	2383	N	GLN	B	354	12.086	17.506	42.178	1.00	26.67	N
ATOM	2384	CA	GLN	B	354	12.580	18.193	43.361	1.00	23.26	C
ATOM	2385	CB	GLN	B	354	11.648	19.339	43.751	1.00	25.56	C
ATOM	2386	CG	GLN	B	354	12.166	20.151	44.923	1.00	30.39	C
ATOM	2387	CD	GLN	B	354	11.363	21.415	45.160	1.00	38.39	C
ATOM	2388	OE1	GLN	B	354	10.625	21.870	44.288	1.00	35.27	O
ATOM	2389	NE2	GLN	B	354	11.523	22.004	46.341	1.00	39.36	N
ATOM	2390	C	GLN	B	354	12.589	17.139	44.470	1.00	27.58	C
ATOM	2391	O	GLN	B	354	11.786	16.188	44.441	1.00	27.31	O
ATOM	2392	N	GLY	B	355	13.496	17.303	45.431	1.00	24.17	N
ATOM	2393	CA	GLY	B	355	13.551	16.367	46.542	1.00	26.73	C
ATOM	2394	C	GLY	B	355	14.388	16.954	47.667	1.00	29.41	C
ATOM	2395	O	GLY	B	355	14.773	18.123	47.626	1.00	24.83	O
ATOM	2396	N	VAL	B	356	14.651	16.125	48.684	1.00	29.40	N
ATOM	2397	CA	VAL	B	356	15.476	16.534	49.817	1.00	27.26	C
ATOM	2398	CB	VAL	B	356	14.633	16.754	51.105	1.00	32.61	C
ATOM	2399	CG1	VAL	B	356	15.549	17.148	52.284	1.00	32.35	C
ATOM	2400	CG2	VAL	B	356	13.611	17.822	50.855	1.00	32.47	C
ATOM	2401	C	VAL	B	356	16.446	15.389	50.059	1.00	21.33	C
ATOM	2402	O	VAL	B	356	16.077	14.233	49.936	1.00	25.09	O
ATOM	2403	N	TYR	B	357	17.690	15.724	50.382	1.00	29.52	N
ATOM	2404	CA	TYR	B	357	18.705	14.706	50.643	1.00	30.43	C
ATOM	2405	CB	TYR	B	357	19.852	14.784	49.631	1.00	35.80	C
ATOM	2406	CG	TYR	B	357	20.948	13.782	49.918	1.00	33.13	C
ATOM	2407	CD1	TYR	B	357	20.784	12.426	49.633	1.00	34.25	C
ATOM	2408	CE1	TYR	B	357	21.789	11.496	49.933	1.00	38.44	C

ATOM	2409	CD2	TYR	B	357	22.135	14.192	50.510	1.00	40.34	C
ATOM	2410	CE2	TYR	B	357	23.143	13.274	50.816	1.00	39.74	C
ATOM	2411	CZ	TYR	B	357	22.964	11.935	50.524	1.00	39.72	C
ATOM	2412	OH	TYR	B	357	23.971	11.048	50.819	1.00	49.57	O
ATOM	2413	C	TYR	B	357	19.266	14.944	52.034	1.00	33.64	C
ATOM	2414	O	TYR	B	357	19.528	16.085	52.420	1.00	32.19	O
ATOM	2415	N	ARG	B	358	19.461	13.863	52.777	1.00	39.19	N
ATOM	2416	CA	ARG	B	358	19.975	13.990	54.133	1.00	42.57	C
ATOM	2417	CB	ARG	B	358	19.248	13.003	55.061	1.00	40.77	C
ATOM	2418	CG	ARG	B	358	19.743	13.027	56.509	1.00	46.82	C
ATOM	2419	CD	ARG	B	358	18.942	12.054	57.364	1.00	45.02	C
ATOM	2420	NE	ARG	B	358	18.989	10.695	56.828	1.00	44.71	N
ATOM	2421	CZ	ARG	B	358	18.075	9.765	57.089	1.00	45.22	C
ATOM	2422	NH1	ARG	B	358	17.048	10.048	57.875	1.00	46.71	N
ATOM	2423	NH2	ARG	B	358	18.184	8.548	56.564	1.00	47.43	N
ATOM	2424	C	ARG	B	358	21.475	13.760	54.228	1.00	37.12	C
ATOM	2425	O	ARG	B	358	21.957	12.680	53.901	1.00	38.27	O
ATOM	2426	N	MET	B	359	22.198	14.798	54.643	1.00	48.39	N
ATOM	2427	CA	MET	B	359	23.641	14.713	54.854	1.00	52.85	C
ATOM	2428	CB	MET	B	359	24.368	15.892	54.211	1.00	56.92	C
ATOM	2429	CG	MET	B	359	24.070	16.084	52.741	1.00	60.92	C
ATOM	2430	SD	MET	B	359	25.113	17.339	51.987	1.00	69.39	S
ATOM	2431	CE	MET	B	359	24.465	18.838	52.768	1.00	66.46	C
ATOM	2432	C	MET	B	359	23.745	14.820	56.371	1.00	57.53	C
ATOM	2433	O	MET	B	359	23.423	15.866	56.936	1.00	66.72	O
ATOM	2434	N	ARG	B	360	24.163	13.741	57.024	1.00	61.83	N
ATOM	2435	CA	ARG	B	360	24.269	13.706	58.488	1.00	63.23	C
ATOM	2436	CB	ARG	B	360	25.166	12.537	58.925	1.00	63.83	C
ATOM	2437	CG	ARG	B	360	24.590	11.170	58.552	1.00	65.58	C
ATOM	2438	CD	ARG	B	360	23.197	11.000	59.158	1.00	65.50	C
ATOM	2439	NE	ARG	B	360	22.294	10.220	58.310	1.00	64.72	N
ATOM	2440	CZ	ARG	B	360	22.467	8.936	57.995	1.00	63.90	C
ATOM	2441	NH1	ARG	B	360	23.523	8.261	58.451	1.00	62.73	N
ATOM	2442	NH2	ARG	B	360	21.573	8.317	57.233	1.00	62.15	N
ATOM	2443	C	ARG	B	360	24.765	15.008	59.099	1.00	61.92	C
ATOM	2444	O	ARG	B	360	25.971	15.181	59.320	1.00	68.74	O
ATOM	2445	N	LYS	B	361	23.811	15.905	59.374	1.00	58.30	N
ATOM	2446	CA	LYS	B	361	24.045	17.233	59.948	1.00	55.64	C
ATOM	2447	CB	LYS	B	361	25.338	17.844	59.389	1.00	60.30	C
ATOM	2448	CG	LYS	B	361	25.334	18.061	57.877	1.00	60.80	C
ATOM	2449	CD	LYS	B	361	26.738	18.379	57.338	1.00	63.13	C
ATOM	2450	CE	LYS	B	361	27.334	19.641	57.964	1.00	63.56	C
ATOM	2451	NZ	LYS	B	361	28.715	19.918	57.453	1.00	66.04	N
ATOM	2452	C	LYS	B	361	22.857	18.139	59.589	1.00	60.03	C
ATOM	2453	O	LYS	B	361	22.408	18.968	60.395	1.00	59.15	O
ATOM	2454	N	LYS	B	362	22.353	17.971	58.365	1.00	53.10	N
ATOM	2455	CA	LYS	B	362	21.225	18.756	57.878	1.00	55.57	C
ATOM	2456	CB	LYS	B	362	21.661	20.202	57.665	1.00	57.57	C
ATOM	2457	CG	LYS	B	362	22.780	20.355	56.656	1.00	54.04	C
ATOM	2458	CD	LYS	B	362	23.226	21.799	56.608	1.00	58.13	C
ATOM	2459	CE	LYS	B	362	24.111	22.049	55.408	1.00	60.20	C
ATOM	2460	NZ	LYS	B	362	25.278	21.126	55.386	1.00	60.23	N
ATOM	2461	C	LYS	B	362	20.659	18.192	56.571	1.00	48.43	C
ATOM	2462	O	LYS	B	362	21.259	17.329	55.945	1.00	47.21	O
ATOM	2463	N	GLN	B	363	19.490	18.675	56.168	1.00	51.49	N
ATOM	2464	CA	GLN	B	363	18.877	18.200	54.935	1.00	49.86	C
ATOM	2465	CB	GLN	B	363	17.463	17.662	55.190	1.00	56.81	C
ATOM	2466	CG	GLN	B	363	17.400	16.534	56.212	1.00	54.91	C
ATOM	2467	CD	GLN	B	363	16.007	15.927	56.325	1.00	55.16	C
ATOM	2468	OE1	GLN	B	363	15.000	16.600	56.098	1.00	61.00	O
ATOM	2469	NE2	GLN	B	363	15.947	14.658	56.692	1.00	58.13	N
ATOM	2470	C	GLN	B	363	18.824	19.341	53.943	1.00	48.03	C
ATOM	2471	O	GLN	B	363	18.369	20.435	54.261	1.00	50.07	O
ATOM	2472	N	ILE	B	364	19.287	19.079	52.727	1.00	39.54	N
ATOM	2473	CA	ILE	B	364	19.294	20.120	51.725	1.00	40.83	C
ATOM	2474	CB	ILE	B	364	20.699	20.335	51.165	1.00	45.38	C
ATOM	2475	CG2	ILE	B	364	21.653	20.714	52.290	1.00	41.39	C
ATOM	2476	CG1	ILE	B	364	21.174	19.071	50.475	1.00	39.09	C

ATOM	2477	CD1	ILE	B	364	22.299	19.333	49.517	1.00	48.16	C
ATOM	2478	C	ILE	B	364	18.361	19.817	50.574	1.00	36.23	C
ATOM	2479	O	ILE	B	364	18.086	18.656	50.268	1.00	30.72	O
ATOM	2480	N	ASP	B	365	17.875	20.870	49.934	1.00	35.72	N
ATOM	2481	CA	ASP	B	365	16.983	20.700	48.797	1.00	33.63	C
ATOM	2482	CB	ASP	B	365	16.300	22.025	48.483	1.00	37.07	C
ATOM	2483	CG	ASP	B	365	15.425	22.506	49.621	1.00	43.21	C
ATOM	2484	OD1	ASP	B	365	14.589	21.712	50.105	1.00	44.93	O
ATOM	2485	OD2	ASP	B	365	15.576	23.678	50.026	1.00	47.38	O
ATOM	2486	C	ASP	B	365	17.825	20.269	47.590	1.00	29.49	C
ATOM	2487	O	ASP	B	365	18.899	20.819	47.363	1.00	32.88	O
ATOM	2488	N	VAL	B	366	17.340	19.303	46.816	1.00	24.92	N
ATOM	2489	CA	VAL	B	366	18.080	18.847	45.653	1.00	25.63	C
ATOM	2490	CB	VAL	B	366	18.718	17.443	45.885	1.00	22.38	C
ATOM	2491	CG1	VAL	B	366	19.793	17.506	46.993	1.00	22.29	C
ATOM	2492	CG2	VAL	B	366	17.619	16.405	46.205	1.00	24.67	C
ATOM	2493	C	VAL	B	366	17.190	18.731	44.420	1.00	23.28	C
ATOM	2494	O	VAL	B	366	15.974	18.745	44.522	1.00	26.31	O
ATOM	2495	N	ALA	B	367	17.816	18.653	43.250	1.00	23.51	N
ATOM	2496	CA	ALA	B	367	17.091	18.439	42.010	1.00	26.78	C
ATOM	2497	CB	ALA	B	367	17.396	19.567	40.990	1.00	25.36	C
ATOM	2498	C	ALA	B	367	17.639	17.074	41.554	1.00	26.08	C
ATOM	2499	O	ALA	B	367	18.843	16.821	41.602	1.00	30.40	O
ATOM	2500	N	ILE	B	368	16.751	16.192	41.128	1.00	25.61	N
ATOM	2501	CA	ILE	B	368	17.124	14.839	40.735	1.00	25.37	C
ATOM	2502	CB	ILE	B	368	16.365	13.781	41.603	1.00	28.96	C
ATOM	2503	CG2	ILE	B	368	16.853	12.365	41.280	1.00	26.27	C
ATOM	2504	CG1	ILE	B	368	16.580	14.082	43.092	1.00	26.82	C
ATOM	2505	CD1	ILE	B	368	15.300	14.229	43.893	1.00	35.04	C
ATOM	2506	C	ILE	B	368	16.796	14.548	39.284	1.00	23.83	C
ATOM	2507	O	ILE	B	368	15.638	14.575	38.895	1.00	24.17	O
ATOM	2508	N	LYS	B	369	17.820	14.261	38.491	1.00	25.66	N
ATOM	2509	CA	LYS	B	369	17.593	13.923	37.089	1.00	26.48	C
ATOM	2510	CB	LYS	B	369	18.853	14.235	36.278	1.00	26.70	C
ATOM	2511	CG	LYS	B	369	18.727	13.997	34.804	1.00	32.20	C
ATOM	2512	CD	LYS	B	369	20.041	14.364	34.094	1.00	31.43	C
ATOM	2513	CE	LYS	B	369	20.013	13.896	32.654	1.00	37.28	C
ATOM	2514	NZ	LYS	B	369	21.184	14.385	31.848	1.00	31.40	N
ATOM	2515	C	LYS	B	369	17.250	12.429	37.070	1.00	30.56	C
ATOM	2516	O	LYS	B	369	18.079	11.572	37.414	1.00	29.63	O
ATOM	2517	N	VAL	B	370	16.016	12.112	36.703	1.00	28.76	N
ATOM	2518	CA	VAL	B	370	15.553	10.730	36.690	1.00	29.89	C
ATOM	2519	CB	VAL	B	370	14.192	10.594	37.410	1.00	32.92	C
ATOM	2520	CG1	VAL	B	370	13.824	9.133	37.553	1.00	38.36	C
ATOM	2521	CG2	VAL	B	370	14.235	11.289	38.775	1.00	31.30	C
ATOM	2522	C	VAL	B	370	15.391	10.222	35.265	1.00	33.31	C
ATOM	2523	O	VAL	B	370	14.623	10.779	34.484	1.00	33.69	O
ATOM	2524	N	LEU	B	371	16.110	9.166	34.921	1.00	32.83	N
ATOM	2525	CA	LEU	B	371	15.992	8.614	33.580	1.00	37.54	C
ATOM	2526	CB	LEU	B	371	17.164	7.676	33.288	1.00	39.83	C
ATOM	2527	CG	LEU	B	371	18.543	8.328	33.234	1.00	40.84	C
ATOM	2528	CD1	LEU	B	371	19.589	7.261	32.948	1.00	41.39	C
ATOM	2529	CD2	LEU	B	371	18.555	9.402	32.166	1.00	39.76	C
ATOM	2530	C	LEU	B	371	14.675	7.853	33.449	1.00	43.14	C
ATOM	2531	O	LEU	B	371	14.307	7.075	34.339	1.00	39.21	O
ATOM	2532	N	LYS.	B	372	13.978	8.075	32.337	1.00	41.93	N
ATOM	2533	CA	LYS	B	372	12.699	7.420	32.080	1.00	47.49	C
ATOM	2534	CB	LYS	B	372	12.114	7.917	30.756	1.00	49.29	C
ATOM	2535	CG	LYS	B	372	13.009	7.677	29.541	1.00	52.95	C
ATOM	2536	CD	LYS	B	372	12.390	8.257	28.275	1.00	54.13	C
ATOM	2537	CE	LYS	B	372	13.254	7.957	27.057	1.00	57.77	C
ATOM	2538	NZ	LYS	B	372	12.655	8.487	25.796	1.00	61.32	N
ATOM	2539	C	LYS	B	372	12.851	5.900	32.052	1.00	52.52	C
ATOM	2540	O	LYS	B	372	13.951	5.378	31.877	1.00	47.39	O
ATOM	2541	N	GLN	B	373	11.740	5.193	32.238	1.00	59.30	N
ATOM	2542	CA	GLN	B	373	11.755	3.733	32.231	1.00	59.74	C
ATOM	2543	CB	GLN	B	373	10.418	3.197	32.762	1.00	64.02	C
ATOM	2544	CG	GLN	B	373	10.377	1.685	32.981	1.00	66.26	C

ATOM	2545	CD	GLN	B	373	11.342	1.215	34.063	1.00	70.74	C
ATOM	2546	OE1	GLN	B	373	12.562	1.337	33.924	1.00	69.05	O
ATOM	2547	NE2	GLN	B	373	10.795	0.672	35.147	1.00	69.07	N
ATOM	2548	C	GLN	B	373	12.005	3.213	30.811	1.00	61.28	C
ATOM	2549	O	GLN	B	373	11.441	3.728	29.840	1.00	59.36	O
ATOM	2550	N	GLY	B	374	12.863	2.203	30.692	1.00	60.31	N
ATOM	2551	CA	GLY	B	374	13.160	1.645	29.385	1.00	62.87	C
ATOM	2552	C	GLY	B	374	14.425	2.207	28.763	1.00	64.46	C
ATOM	2553	O	GLY	B	374	14.792	1.838	27.643	1.00	64.42	O
ATOM	2554	N	THR	B	375	15.091	3.101	29.490	1.00	62.61	N
ATOM	2555	CA	THR	B	375	16.326	3.722	29.019	1.00	62.15	C
ATOM	2556	CB	THR	B	375	16.913	4.678	30.089	1.00	61.37	C
ATOM	2557	OG1	THR	B	375	16.039	5.799	30.268	1.00	57.85	O
ATOM	2558	CG2	THR	B	375	18.288	5.175	29.671	1.00	61.31	C
ATOM	2559	C	THR	B	375	17.374	2.666	28.673	1.00	60.79	C
ATOM	2560	O	THR	B	375	17.728	1.835	29.507	1.00	61.50	O
ATOM	2561	N	GLU	B	376	17.867	2.708	27.440	1.00	61.17	N
ATOM	2562	CA	GLU	B	376	18.874	1.753	26.990	1.00	63.67	C
ATOM	2563	CB	GLU	B	376	19.139	1.933	25.496	1.00	65.15	C
ATOM	2564	CG	GLU	B	376	20.120	0.923	24.917	1.00	71.18	C
ATOM	2565	CD	GLU	B	376	20.089	0.883	23.398	1.00	73.78	C
ATOM	2566	OE1	GLU	B	376	20.380	1.923	22.758	1.00	72.53	O
ATOM	2567	OE2	GLU	B	376	19.769	-0.193	22.843	1.00	73.05	O
ATOM	2568	C	GLU	B	376	20.169	1.943	27.771	1.00	65.33	C
ATOM	2569	O	GLU	B	376	20.462	3.046	28.237	1.00	61.91	O
ATOM	2570	N	LYS	B	377	20.940	0.868	27.910	1.00	59.58	N
ATOM	2571	CA	LYS	B	377	22.196	0.927	28.644	1.00	61.29	C
ATOM	2572	CB	LYS	B	377	22.896	-0.432	28.608	1.00	65.21	C
ATOM	2573	CG	LYS	B	377	24.222	-0.454	29.356	1.00	65.59	C
ATOM	2574	CD	LYS	B	377	24.611	-1.872	29.736	1.00	71.26	C
ATOM	2575	CE	LYS	B	377	25.867	-1.896	30.599	1.00	70.47	C
ATOM	2576	NZ	LYS	B	377	26.267	-3.292	30.962	1.00	72.53	N
ATOM	2577	C	LYS	B	377	23.131	1.993	28.095	1.00	59.78	C
ATOM	2578	O	LYS	B	377	23.999	2.497	28.808	1.00	56.95	O
ATOM	2579	N	ALA	B	378	22.952	2.329	26.823	1.00	61.07	N
ATOM	2580	CA	ALA	B	378	23.777	3.337	26.168	1.00	59.33	C
ATOM	2581	CB	ALA	B	378	23.399	3.435	24.695	1.00	59.59	C
ATOM	2582	C	ALA	B	378	23.624	4.703	26.836	1.00	57.38	C
ATOM	2583	O	ALA	B	378	24.612	5.376	27.138	1.00	56.25	O
ATOM	2584	N	ASP	B	379	22.380	5.098	27.075	1.00	57.35	N
ATOM	2585	CA	ASP	B	379	22.094	6.388	27.691	1.00	59.15	C
ATOM	2586	CB	ASP	B	379	20.650	6.788	27.416	1.00	61.51	C
ATOM	2587	CG	ASP	B	379	20.151	6.255	26.088	1.00	68.59	C
ATOM	2588	OD1	ASP	B	379	20.739	6.601	25.035	1.00	70.20	O
ATOM	2589	OD2	ASP	B	379	19.168	5.479	26.098	1.00	70.89	O
ATOM	2590	C	ASP	B	379	22.341	6.358	29.197	1.00	56.77	C
ATOM	2591	O	ASP	B	379	22.596	7.392	29.811	1.00	53.33	O
ATOM	2592	N	THR	B	380	22.258	5.170	29.790	1.00	52.16	N
ATOM	2593	CA	THR	B	380	22.513	5.019	31.215	1.00	53.38	C
ATOM	2594	CB	THR	B	380	22.187	3.590	31.684	1.00	53.55	C
ATOM	2595	OG1	THR	B	380	20.768	3.391	31.641	1.00	54.68	O
ATOM	2596	CG2	THR	B	380	22.683	3.371	33.096	1.00	58.07	C
ATOM	2597	C	THR	B	380	23.998	5.295	31.432	1.00	52.60	C
ATOM	2598	O	THR	B	380	24.390	5.980	32.374	1.00	48.13	O
ATOM	2599	N	GLU	B	381	24.819	4.752	30.540	1.00	46.95	N
ATOM	2600	CA	GLU	B	381	26.260	4.937	30.617	1.00	49.11	C
ATOM	2601	CB	GLU	B	381	26.955	4.060	29.573	1.00	54.95	C
ATOM	2602	CG	GLU	B	381	28.020	3.129	30.134	1.00	58.45	C
ATOM	2603	CD	GLU	B	381	27.442	1.927	30.862	1.00	65.92	C
ATOM	2604	OE1	GLU	B	381	26.790	2.114	31.913	1.00	66.10	O
ATOM	2605	OE2	GLU	B	381	27.644	0.788	30.377	1.00	67.00	O
ATOM	2606	C	GLU	B	381	26.559	6.412	30.343	1.00	45.43	C
ATOM	2607	O	GLU	B	381	27.518	6.974	30.864	1.00	40.91	O
ATOM	2608	N	GLU	B	382	25.716	7.029	29.525	1.00	43.34	N
ATOM	2609	CA	GLU	B	382	25.871	8.435	29.164	1.00	45.73	C
ATOM	2610	CB	GLU	B	382	24.842	8.795	28.099	1.00	50.57	C
ATOM	2611	CG	GLU	B	382	24.988	10.184	27.524	1.00	55.43	C
ATOM	2612	CD	GLU	B	382	24.064	10.410	26.336	1.00	60.92	C

ATOM	2613	OE1	GLU	B	382	22.825	10.449	26.528	1.00	67.80	O
ATOM	2614	OE2	GLU	B	382	24.580	10.536	25.203	1.00	65.61	O
ATOM	2615	C	GLU	B	382	25.696	9.331	30.394	1.00	42.57	C
ATOM	2616	O	GLU	B	382	26.444	10.294	30.587	1.00	36.66	O
ATOM	2617	N	MET	B	383	24.700	9.017	31.217	1.00	36.27	N
ATOM	2618	CA	MET	B	383	24.482	9.806	32.417	1.00	36.21	C
ATOM	2619	CB	MET	B	383	23.116	9.489	33.051	1.00	37.94	C
ATOM	2620	CG	MET	B	383	22.686	10.580	34.040	1.00	45.05	C
ATOM	2621	SD	MET	B	383	21.039	10.380	34.734	1.00	49.17	S
ATOM	2622	CE	MET	B	383	21.377	9.057	35.776	1.00	31.72	C
ATOM	2623	C	MET	B	383	25.602	9.543	33.420	1.00	32.29	C
ATOM	2624	O	MET	B	383	25.912	10.389	34.245	1.00	27.76	O
ATOM	2625	N	MET	B	384	26.212	8.361	33.362	1.00	32.45	N
ATOM	2626	CA	MET	B	384	27.310	8.076	34.276	1.00	34.42	C
ATOM	2627	CB	MET	B	384	27.664	6.588	34.262	1.00	38.83	C
ATOM	2628	CG	MET	B	384	26.634	5.702	34.943	1.00	41.15	C
ATOM	2629	SD	MET	B	384	26.295	6.179	36.672	1.00	47.37	S
ATOM	2630	CE	MET	B	384	27.936	6.041	37.407	1.00	46.98	C
ATOM	2631	C	MET	B	384	28.529	8.911	33.896	1.00	31.48	C
ATOM	2632	O	MET	B	384	29.284	9.352	34.762	1.00	31.65	O
ATOM	2633	N	ARG	B	385	28.727	9.133	32.603	1.00	34.67	N
ATOM	2634	CA	ARG	B	385	29.848	9.962	32.172	1.00	36.33	C
ATOM	2635	CB	ARG	B	385	30.011	9.926	30.652	1.00	37.82	C
ATOM	2636	CG	ARG	B	385	30.687	8.667	30.129	1.00	45.45	C
ATOM	2637	CD	ARG	B	385	31.105	8.837	28.665	1.00	46.60	C
ATOM	2638	NE	ARG	B	385	29.969	8.752	27.756	1.00	45.85	N
ATOM	2639	CZ	ARG	B	385	29.377	7.610	27.417	1.00	47.08	C
ATOM	2640	NH1	ARG	B	385	29.823	6.459	27.913	1.00	48.61	N
ATOM	2641	NH2	ARG	B	385	28.342	7.612	26.592	1.00	46.74	N
ATOM	2642	C	ARG	B	385	29.596	11.391	32.636	1.00	29.96	C
ATOM	2643	O	ARG	B	385	30.520	12.098	33.021	1.00	33.63	O
ATOM	2644	N	GLU	B	386	28.330	11.799	32.612	1.00	30.00	N
ATOM	2645	CA	GLU	B	386	27.948	13.141	33.051	1.00	29.80	C
ATOM	2646	CB	GLU	B	386	26.447	13.368	32.790	1.00	27.12	C
ATOM	2647	CG	GLU	B	386	25.882	14.720	33.233	1.00	32.18	C
ATOM	2648	CD	GLU	B	386	24.372	14.825	32.961	1.00	35.05	C
ATOM	2649	OE1	GLU	B	386	23.801	13.830	32.475	1.00	34.50	O
ATOM	2650	OE2	GLU	B	386	23.756	15.890	33.251	1.00	35.81	O
ATOM	2651	C	GLU	B	386	28.259	13.298	34.540	1.00	28.79	C
ATOM	2652	O	GLU	B	386	28.752	14.350	34.986	1.00	26.92	O
ATOM	2653	N	ALA	B	387	27.967	12.253	35.305	1.00	30.29	N
ATOM	2654	CA	ALA	B	387	28.223	12.295	36.736	1.00	33.27	C
ATOM	2655	CB	ALA	B	387	27.644	11.044	37.421	1.00	30.95	C
ATOM	2656	C	ALA	B	387	29.744	12.398	36.962	1.00	26.41	C
ATOM	2657	O	ALA	B	387	30.191	13.182	37.774	1.00	35.19	O
ATOM	2658	N	GLN	B	388	30.518	11.614	36.219	1.00	32.50	N
ATOM	2659	CA	GLN	B	388	31.984	11.654	36.367	1.00	37.92	C
ATOM	2660	CB	GLN	B	388	32.647	10.664	35.387	1.00	38.99	C
ATOM	2661	CG	GLN	B	388	32.269	9.211	35.625	1.00	47.85	C
ATOM	2662	CD	GLN	B	388	32.810	8.279	34.546	1.00	56.30	C
ATOM	2663	OE1	GLN	B	388	34.016	8.248	34.281	1.00	56.71	O
ATOM	2664	NE2	GLN	B	388	31.914	7.514	33.915	1.00	53.14	N
ATOM	2665	C	GLN	B	388	32.546	13.060	36.134	1.00	35.03	C
ATOM	2666	O	GLN	B	388	33.442	13.501	36.841	1.00	32.27	O
ATOM	2667	N	ILE	B	389	32.015	13.767	35.135	1.00	30.85	N
ATOM	2668	CA	ILE	B	389	32.463	15.130	34.840	1.00	25.41	C
ATOM	2669	CB	ILE	B	389	31.853	15.645	33.499	1.00	32.74	C
ATOM	2670	CG2	ILE	B	389	32.051	17.159	33.363	1.00	31.69	C
ATOM	2671	CG1	ILE	B	389	32.505	14.906	32.328	1.00	38.87	C
ATOM	2672	CD1	ILE	B	389	31.893	15.236	30.982	1.00	36.36	C
ATOM	2673	C	ILE	B	389	32.072	16.074	35.949	1.00	26.93	C
ATOM	2674	O	ILE	B	389	32.872	16.886	36.411	1.00	30.11	O
ATOM	2675	N	MET	B	390	30.832	15.978	36.403	1.00	26.48	N
ATOM	2676	CA	MET	B	390	30.398	16.857	37.459	1.00	24.57	C
ATOM	2677	CB	MET	B	390	28.906	16.695	37.735	1.00	24.91	C
ATOM	2678	CG	MET	B	390	28.002	17.248	36.638	1.00	26.56	C
ATOM	2679	SD	MET	B	390	26.239	17.032	37.117	1.00	30.07	S
ATOM	2680	CE	MET	B	390	26.009	18.455	38.144	1.00	31.13	C

ATOM	2681	C	MET	B	390	31.186	16.563	38.738	1.00	30.37	C
ATOM	2682	O	MET	B	390	31.506	17.484	39.487	1.00	29.10	O
ATOM	2683	N	HIS	B	391	31.497	15.286	38.956	1.00	31.09	N
ATOM	2684	CA	HIS	B	391	32.243	14.890	40.160	1.00	37.62	C
ATOM	2685	CB	HIS	B	391	32.285	13.358	40.270	1.00	42.66	C
ATOM	2686	CG	HIS	B	391	32.831	12.854	41.573	1.00	50.59	C
ATOM	2687	CD2	HIS	B	391	32.206	12.397	42.686	1.00	51.17	C
ATOM	2688	ND1	HIS	B	391	34.182	12.815	41.850	1.00	56.54	N
ATOM	2689	CE1	HIS	B	391	34.366	12.356	43.076	1.00	56.46	C
ATOM	2690	NE2	HIS	B	391	33.183	12.094	43.605	1.00	57.11	N
ATOM	2691	C	HIS	B	391	33.661	15.454	40.155	1.00	43.32	C
ATOM	2692	O	HIS	B	391	34.338	15.452	41.182	1.00	47.18	O
ATOM	2693	N	GLN	B	392	34.111	15.941	38.999	1.00	39.89	N
ATOM	2694	CA	GLN	B	392	35.449	16.516	38.886	1.00	40.61	C
ATOM	2695	CB	GLN	B	392	36.094	16.110	37.557	1.00	42.86	C
ATOM	2696	CG	GLN	B	392	36.181	14.610	37.364	1.00	47.64	C
ATOM	2697	CD	GLN	B	392	36.948	14.219	36.129	1.00	50.73	C
ATOM	2698	OE1	GLN	B	392	38.161	14.408	36.058	1.00	60.38	O
ATOM	2699	NE2	GLN	B	392	36.250	13.664	35.145	1.00	48.83	N
ATOM	2700	C	GLN	B	392	35.415	18.031	38.987	1.00	47.76	C
ATOM	2701	O	GLN	B	392	36.444	18.689	38.850	1.00	46.42	O
ATOM	2702	N	LEU	B	393	34.233	18.586	39.240	1.00	45.72	N
ATOM	2703	CA	LEU	B	393	34.069	20.034	39.342	1.00	45.69	C
ATOM	2704	CB	LEU	B	393	32.909	20.491	38.454	1.00	44.69	C
ATOM	2705	CG	LEU	B	393	32.913	20.011	37.000	1.00	46.90	C
ATOM	2706	CD1	LEU	B	393	31.656	20.508	36.312	1.00	44.79	C
ATOM	2707	CD2	LEU	B	393	34.153	20.507	36.281	1.00	37.05	C
ATOM	2708	C	LEU	B	393	33.826	20.515	40.770	1.00	45.06	C
ATOM	2709	O	LEU	B	393	33.044	19.928	41.523	1.00	49.45	O
ATOM	2710	N	ASP	B	394	34.481	21.603	41.151	1.00	43.03	N
ATOM	2711	CA	ASP	B	394	34.315	22.133	42.495	1.00	36.00	C
ATOM	2712	CB	ASP	B	394	35.432	21.600	43.403	1.00	47.00	C
ATOM	2713	CG	ASP	B	394	35.292	22.063	44.844	1.00	52.54	C
ATOM	2714	OD1	ASP	B	394	36.167	21.705	45.668	1.00	55.59	O
ATOM	2715	OD2	ASP	B	394	34.315	22.774	45.160	1.00	47.08	O
ATOM	2716	C	ASP	B	394	34.381	23.640	42.427	1.00	40.50	C
ATOM	2717	O	ASP	B	394	35.434	24.247	42.671	1.00	38.62	O
ATOM	2718	N	ASN	B	395	33.251	24.254	42.105	1.00	35.95	N
ATOM	2719	CA	ASN	B	395	33.216	25.699	41.987	1.00	31.17	C
ATOM	2720	CB	ASN	B	395	33.463	26.092	40.518	1.00	25.15	C
ATOM	2721	CG	ASN	B	395	33.595	27.578	40.328	1.00	36.48	C
ATOM	2722	OD1	ASN	B	395	34.673	28.158	40.523	1.00	37.23	O
ATOM	2723	ND2	ASN	B	395	32.497	28.217	39.950	1.00	25.99	N
ATOM	2724	C	ASN	B	395	31.851	26.171	42.458	1.00	30.67	C
ATOM	2725	O	ASN	B	395	30.821	25.528	42.197	1.00	28.65	O
ATOM	2726	N	PRO	B	396	31.822	27.315	43.147	1.00	27.83	N
ATOM	2727	CD	PRO	B	396	32.966	28.068	43.680	1.00	37.81	C
ATOM	2728	CA	PRO	B	396	30.570	27.867	43.655	1.00	26.99	C
ATOM	2729	CB	PRO	B	396	31.036	29.053	44.483	1.00	35.20	C
ATOM	2730	CG	PRO	B	396	32.414	28.620	44.946	1.00	41.91	C
ATOM	2731	C	PRO	B	396	29.568	28.291	42.579	1.00	29.09	C
ATOM	2732	O	PRO	B	396	28.402	28.428	42.865	1.00	26.93	O
ATOM	2733	N	TYR	B	397	30.043	28.485	41.343	1.00	24.67	N
ATOM	2734	CA	TYR	B	397	29.145	28.956	40.263	1.00	24.00	C
ATOM	2735	CB	TYR	B	397	29.827	30.136	39.545	1.00	23.32	C
ATOM	2736	CG	TYR	B	397	30.228	31.229	40.524	1.00	26.27	C
ATOM	2737	CD1	TYR	B	397	31.568	31.425	40.881	1.00	26.92	C
ATOM	2738	CE1	TYR	B	397	31.929	32.379	41.823	1.00	31.33	C
ATOM	2739	CD2	TYR	B	397	29.266	32.024	41.136	1.00	25.87	C
ATOM	2740	CE2	TYR	B	397	29.620	32.987	42.085	1.00	33.47	C
ATOM	2741	CZ	TYR	B	397	30.950	33.155	42.426	1.00	34.44	C
ATOM	2742	OH	TYR	B	397	31.263	34.067	43.411	1.00	37.25	O
ATOM	2743	C	TYR	B	397	28.694	27.893	39.294	1.00	23.67	C
ATOM	2744	O	TYR	B	397	28.286	28.165	38.135	1.00	24.69	O
ATOM	2745	N	ILE	B	398	28.755	26.659	39.752	1.00	21.85	N
ATOM	2746	CA	ILE	B	398	28.336	25.519	38.991	1.00	26.71	C
ATOM	2747	CB	ILE	B	398	29.567	24.716	38.567	1.00	34.69	C
ATOM	2748	CG2	ILE	B	398	29.165	23.359	38.073	1.00	36.71	C

ATOM	2749	CG1	ILE	B	398	30.332	25.501	37.498	1.00	28.39	C
ATOM	2750	CD1	ILE	B	398	31.737	25.021	37.232	1.00	39.03	C
ATOM	2751	C	ILE	B	398	27.421	24.691	39.906	1.00	34.83	C
ATOM	2752	O	ILE	B	398	27.640	24.636	41.120	1.00	31.60	O
ATOM	2753	N	VAL	B	399	26.378	24.103	39.333	1.00	26.19	N
ATOM	2754	CA	VAL	B	399	25.458	23.243	40.086	1.00	29.92	C
ATOM	2755	CB	VAL	B	399	24.272	22.781	39.232	1.00	30.42	C
ATOM	2756	CG1	VAL	B	399	23.498	21.627	39.946	1.00	29.50	C
ATOM	2757	CG2	VAL	B	399	23.360	23.960	38.970	1.00	31.26	C
ATOM	2758	C	VAL	B	399	26.265	22.016	40.464	1.00	34.54	C
ATOM	2759	O	VAL	B	399	26.697	21.269	39.597	1.00	35.65	O
ATOM	2760	N	ARG	B	400	26.430	21.805	41.763	1.00	27.76	N
ATOM	2761	CA	ARG	B	400	27.227	20.683	42.244	1.00	32.53	C
ATOM	2762	CB	ARG	B	400	27.744	20.994	43.658	1.00	38.09	C
ATOM	2763	CG	ARG	B	400	28.606	22.262	43.787	1.00	46.29	C
ATOM	2764	CD	ARG	B	400	28.970	22.541	45.262	1.00	46.35	C
ATOM	2765	NE	ARG	B	400	29.833	23.711	45.437	1.00	52.96	N
ATOM	2766	CZ	ARG	B	400	31.116	23.743	45.092	1.00	55.68	C
ATOM	2767	NH1	ARG	B	400	31.675	22.666	44.557	1.00	51.73	N
ATOM	2768	NH2	ARG	B	400	31.841	24.847	45.278	1.00	52.56	N
ATOM	2769	C	ARG	B	400	26.513	19.345	42.256	1.00	27.44	C
ATOM	2770	O	ARG	B	400	25.313	19.254	42.507	1.00	28.50	O
ATOM	2771	N	LEU	B	401	27.259	18.280	42.006	1.00	27.68	N
ATOM	2772	CA	LEU	B	401	26.695	16.948	42.018	1.00	24.03	C
ATOM	2773	CB	LEU	B	401	27.514	16.006	41.156	1.00	32.24	C
ATOM	2774	CG	LEU	B	401	27.086	14.540	41.184	1.00	29.66	C
ATOM	2775	CD1	LEU	B	401	25.713	14.354	40.554	1.00	35.88	C
ATOM	2776	CD2	LEU	B	401	28.132	13.737	40.425	1.00	39.27	C
ATOM	2777	C	LEU	B	401	26.745	16.426	43.456	1.00	35.79	C
ATOM	2778	O	LEU	B	401	27.796	16.487	44.103	1.00	29.49	O
ATOM	2779	N	ILE	B	402	25.611	15.945	43.957	1.00	27.95	N
ATOM	2780	CA	ILE	B	402	25.581	15.368	45.299	1.00	29.27	C
ATOM	2781	CB	ILE	B	402	24.154	15.383	45.922	1.00	31.13	C
ATOM	2782	CG2	ILE	B	402	24.188	14.716	47.305	1.00	33.30	C
ATOM	2783	CG1	ILE	B	402	23.650	16.830	46.065	1.00	26.94	C
ATOM	2784	CD1	ILE	B	402	24.616	17.763	46.743	1.00	31.79	C
ATOM	2785	C	ILE	B	402	26.053	13.921	45.119	1.00	32.38	C
ATOM	2786	O	ILE	B	402	26.962	13.448	45.812	1.00	31.53	O
ATOM	2787	N	GLY	B	403	25.469	13.226	44.157	1.00	27.83	N
ATOM	2788	CA	GLY	B	403	25.870	11.853	43.900	1.00	29.46	C
ATOM	2789	C	GLY	B	403	24.897	11.150	42.994	1.00	29.35	C
ATOM	2790	O	GLY	B	403	23.934	11.757	42.537	1.00	30.33	O
ATOM	2791	N	VAL	B	404	25.145	9.878	42.717	1.00	26.15	N
ATOM	2792	CA	VAL	B	404	24.281	9.084	41.865	1.00	28.12	C
ATOM	2793	CB	VAL	B	404	25.106	8.273	40.844	1.00	36.04	C
ATOM	2794	CG1	VAL	B	404	24.186	7.397	39.982	1.00	40.40	C
ATOM	2795	CG2	VAL	B	404	25.911	9.211	39.982	1.00	35.87	C
ATOM	2796	C	VAL	B	404	23.519	8.114	42.755	1.00	32.26	C
ATOM	2797	O	VAL	B	404	24.052	7.647	43.744	1.00	31.47	O
ATOM	2798	N	CYS	B	405	22.277	7.815	42.392	1.00	30.13	N
ATOM	2799	CA	CYS	B	405	21.471	6.879	43.177	1.00	35.84	C
ATOM	2800	CB	CYS	B	405	20.408	7.635	43.976	1.00	39.61	C
ATOM	2801	SG	CYS	B	405	19.571	6.617	45.215	1.00	43.65	S
ATOM	2802	C	CYS	B	405	20.815	5.849	42.258	1.00	41.06	C
ATOM	2803	O	CYS	B	405	20.101	6.200	41.320	1.00	38.70	O
ATOM	2804	N	GLN	B	406	21.086	4.577	42.510	1.00	41.04	N
ATOM	2805	CA	GLN	B	406	20.529	3.511	41.687	1.00	49.92	C
ATOM	2806	CB	GLN	B	406	21.639	2.549	41.250	1.00	53.55	C
ATOM	2807	CG	GLN	B	406	21.165	1.355	40.413	1.00	59.57	C
ATOM	2808	CD	GLN	B	406	20.378	1.756	39.169	1.00	56.22	C
ATOM	2809	OE1	GLN	B	406	19.205	2.123	39.246	1.00	59.42	O
ATOM	2810	NE2	GLN	B	406	21.028	1.687	38.016	1.00	59.35	N
ATOM	2811	C	GLN	B	406	19.450	2.750	42.446	1.00	53.55	C
ATOM	2812	O	GLN	B	406	19.746	1.894	43.273	1.00	56.70	O
ATOM	2813	N	ALA	B	407	18.197	3.080	42.163	1.00	56.23	N
ATOM	2814	CA	ALA	B	407	17.069	2.418	42.808	1.00	60.79	C
ATOM	2815	CB	ALA	B	407	16.432	3.359	43.829	1.00	60.88	C
ATOM	2816	C	ALA	B	407	16.052	2.012	41.742	1.00	58.91	C

ATOM	2817	O	ALA	B	407	16.364	1.212	40.856	1.00	57.00	O
ATOM	2818	N	GLU	B	408	14.846	2.568	41.821	1.00	55.11	N
ATOM	2819	CA	GLU	B	408	13.806	2.260	40.849	1.00	57.75	C
ATOM	2820	CB	GLU	B	408	12.535	3.065	41.147	1.00	61.87	C
ATOM	2821	CG	GLU	B	408	12.759	4.562	41.299	1.00	61.03	C
ATOM	2822	CD	GLU	B	408	12.938	4.998	42.748	1.00	61.45	C
ATOM	2823	OE1	GLU	B	408	13.788	4.422	43.464	1.00	62.30	O
ATOM	2824	OE2	GLU	B	408	12.228	5.933	43.169	1.00	57.96	O
ATOM	2825	C	GLU	B	408	14.320	2.590	39.452	1.00	58.74	C
ATOM	2826	O	GLU	B	408	13.770	2.139	38.444	1.00	61.01	O
ATOM	2827	N	ALA	B	409	15.383	3.387	39.408	1.00	58.64	N
ATOM	2828	CA	ALA	B	409	16.017	3.788	38.159	1.00	53.23	C
ATOM	2829	CB	ALA	B	409	15.054	4.621	37.327	1.00	57.75	C
ATOM	2830	C	ALA	B	409	17.262	4.595	38.518	1.00	48.64	C
ATOM	2831	O	ALA	B	409	17.451	4.957	39.682	1.00	41.77	O
ATOM	2832	N	LEU	B	410	18.113	4.859	37.527	1.00	46.67	N
ATOM	2833	CA	LEU	B	410	19.348	5.606	37.757	1.00	41.56	C
ATOM	2834	CB	LEU	B	410	20.326	5.370	36.607	1.00	41.30	C
ATOM	2835	CG	LEU	B	410	21.745	5.849	36.893	1.00	39.49	C
ATOM	2836	CD1	LEU	B	410	22.282	5.132	38.127	1.00	40.07	C
ATOM	2837	CD2	LEU	B	410	22.628	5.590	35.680	1.00	44.22	C
ATOM	2838	C	LEU	B	410	19.024	7.087	37.877	1.00	36.27	C
ATOM	2839	O	LEU	B	410	18.291	7.631	37.068	1.00	32.58	O
ATOM	2840	N	MET	B	411	19.579	7.740	38.888	1.00	31.99	N
ATOM	2841	CA	MET	B	411	19.277	9.144	39.105	1.00	28.85	C
ATOM	2842	CB	MET	B	411	18.272	9.282	40.261	1.00	27.82	C
ATOM	2843	CG	MET	B	411	16.998	8.467	40.120	1.00	38.03	C
ATOM	2844	SD	MET	B	411	15.902	8.655	41.550	1.00	39.66	S
ATOM	2845	CE	MET	B	411	16.875	7.893	42.769	1.00	39.08	C
ATOM	2846	C	MET	B	411	20.518	9.931	39.454	1.00	34.64	C
ATOM	2847	O	MET	B	411	21.415	9.412	40.110	1.00	32.86	O
ATOM	2848	N	LEU	B	412	20.576	11.182	39.012	1.00	27.07	N
ATOM	2849	CA	LEU	B	412	21.686	12.070	39.353	1.00	24.70	C
ATOM	2850	CB	LEU	B	412	22.213	12.819	38.122	1.00	31.40	C
ATOM	2851	CG	LEU	B	412	23.072	12.039	37.146	1.00	42.38	C
ATOM	2852	CD1	LEU	B	412	23.695	13.008	36.127	1.00	40.09	C
ATOM	2853	CD2	LEU	B	412	24.156	11.325	37.940	1.00	44.83	C
ATOM	2854	C	LEU	B	412	21.108	13.086	40.316	1.00	32.72	C
ATOM	2855	O	LEU	B	412	20.203	13.829	39.930	1.00	25.93	O
ATOM	2856	N	VAL	B	413	21.632	13.118	41.552	1.00	25.13	N
ATOM	2857	CA	VAL	B	413	21.179	14.048	42.591	1.00	22.67	C
ATOM	2858	CB	VAL	B	413	21.169	13.374	43.997	1.00	27.42	C
ATOM	2859	CG1	VAL	B	413	20.591	14.333	45.040	1.00	22.22	C
ATOM	2860	CG2	VAL	B	413	20.369	12.079	43.932	1.00	27.93	C
ATOM	2861	C	VAL	B	413	22.099	15.245	42.627	1.00	26.70	C
ATOM	2862	O	VAL	B	413	23.317	15.115	42.869	1.00	28.13	O
ATOM	2863	N	MET	B	414	21.503	16.417	42.414	1.00	23.91	N
ATOM	2864	CA	MET	B	414	22.232	17.672	42.353	1.00	23.05	C
ATOM	2865	CB	MET	B	414	22.146	18.241	40.913	1.00	26.27	C
ATOM	2866	CG	MET	B	414	22.782	17.373	39.850	1.00	31.80	C
ATOM	2867	SD	MET	B	414	22.187	17.909	38.179	1.00	31.87	S
ATOM	2868	CE	MET	B	414	20.682	16.914	38.038	1.00	34.99	C
ATOM	2869	C	MET	B	414	21.683	18.729	43.269	1.00	24.82	C
ATOM	2870	O	MET	B	414	20.536	18.646	43.732	1.00	26.89	O
ATOM	2871	N	GLU	B	415	22.475	19.767	43.508	1.00	22.82	N
ATOM	2872	CA	GLU	B	415	22.008	20.867	44.330	1.00	25.46	C
ATOM	2873	CB	GLU	B	415	23.089	21.939	44.500	1.00	38.09	C
ATOM	2874	CG	GLU	B	415	24.381	21.466	45.121	1.00	41.76	C
ATOM	2875	CD	GLU	B	415	25.406	22.600	45.191	1.00	56.15	C
ATOM	2876	OE1	GLU	B	415	25.611	23.293	44.153	1.00	43.26	O
ATOM	2877	OE2	GLU	B	415	26.000	22.796	46.279	1.00	53.48	O
ATOM	2878	C	GLU	B	415	20.848	21.511	43.581	1.00	28.34	C
ATOM	2879	O	GLU	B	415	20.819	21.496	42.347	1.00	27.84	O
ATOM	2880	N	MET	B	416	19.903	22.079	44.327	1.00	28.24	N
ATOM	2881	CA	MET	B	416	18.776	22.739	43.701	1.00	27.37	C
ATOM	2882	CB	MET	B	416	17.482	22.444	44.452	1.00	31.26	C
ATOM	2883	CG	MET	B	416	16.245	22.889	43.658	1.00	33.79	C
ATOM	2884	SD	MET	B	416	14.717	22.640	44.566	1.00	40.24	S

ATOM	2885	CE	MET	B	416	13.622	23.863	43.732	1.00	41.28	C
ATOM	2886	C	MET	B	416	18.989	24.247	43.709	1.00	32.53	C
ATOM	2887	O	MET	B	416	19.462	24.797	44.695	1.00	29.31	O
ATOM	2888	N	ALA	B	417	18.639	24.900	42.603	1.00	29.63	N
ATOM	2889	CA	ALA	B	417	18.724	26.362	42.497	1.00	32.11	C
ATOM	2890	CB	ALA	B	417	19.676	26.775	41.365	1.00	31.26	C
ATOM	2891	C	ALA	B	417	17.282	26.779	42.186	1.00	32.20	C
ATOM	2892	O	ALA	B	417	16.903	26.933	41.017	1.00	31.90	O
ATOM	2893	N	GLY	B	418	16.500	26.924	43.259	1.00	34.38	N
ATOM	2894	CA	GLY	B	418	15.081	27.243	43.183	1.00	36.34	C
ATOM	2895	C	GLY	B	418	14.630	28.461	42.398	1.00	34.85	C
ATOM	2896	O	GLY	B	418	13.447	28.598	42.082	1.00	34.44	O
ATOM	2897	N	GLY	B	419	15.563	29.359	42.105	1.00	28.57	N
ATOM	2898	CA	GLY	B	419	15.208	30.537	41.339	1.00	30.78	C
ATOM	2899	C	GLY	B	419	14.891	30.180	39.897	1.00	33.81	C
ATOM	2900	O	GLY	B	419	14.245	30.944	39.202	1.00	32.35	O
ATOM	2901	N	GLY	B	420	15.370	29.032	39.427	1.00	30.29	N
ATOM	2902	CA	GLY	B	420	15.091	28.621	38.065	1.00	27.83	C
ATOM	2903	C	GLY	B	420	15.930	29.299	36.980	1.00	24.88	C
ATOM	2904	O	GLY	B	420	16.843	30.054	37.303	1.00	24.54	O
ATOM	2905	N	PRO	B	421	15.617	29.068	35.694	1.00	26.97	N
ATOM	2906	CD	PRO	B	421	14.445	28.280	35.256	1.00	26.58	C
ATOM	2907	CA	PRO	B	421	16.320	29.631	34.534	1.00	26.79	C
ATOM	2908	CB	PRO	B	421	15.508	29.113	33.335	1.00	31.97	C
ATOM	2909	CG	PRO	B	421	14.810	27.921	33.845	1.00	32.59	C
ATOM	2910	C	PRO	B	421	16.400	31.148	34.507	1.00	31.93	C
ATOM	2911	O	PRO	B	421	15.430	31.851	34.801	1.00	26.82	O
ATOM	2912	N	LEU	B	422	17.570	31.643	34.112	1.00	24.30	N
ATOM	2913	CA	LEU	B	422	17.848	33.064	34.025	1.00	25.19	C
ATOM	2914	CB	LEU	B	422	19.316	33.263	33.632	1.00	26.63	C
ATOM	2915	CG	LEU	B	422	19.835	34.685	33.470	1.00	27.37	C
ATOM	2916	CD1	LEU	B	422	19.814	35.394	34.801	1.00	28.60	C
ATOM	2917	CD2	LEU	B	422	21.251	34.623	32.917	1.00	25.74	C
ATOM	2918	C	LEU	B	422	16.966	33.799	33.003	1.00	22.35	C
ATOM	2919	O	LEU	B	422	16.524	34.916	33.268	1.00	27.34	O
ATOM	2920	N	HIS	B	423	16.753	33.207	31.835	1.00	23.59	N
ATOM	2921	CA	HIS	B	423	15.944	33.884	30.829	1.00	33.17	C
ATOM	2922	CB	HIS	B	423	15.899	33.099	29.518	1.00	33.79	C
ATOM	2923	CG	HIS	B	423	15.322	31.725	29.650	1.00	30.44	C
ATOM	2924	CD2	HIS	B	423	15.309	30.856	30.688	1.00	33.89	C
ATOM	2925	ND1	HIS	B	423	14.631	31.109	28.626	1.00	40.96	N
ATOM	2926	CE1	HIS	B	423	14.222	29.919	29.029	1.00	35.92	C
ATOM	2927	NE2	HIS	B	423	14.621	29.740	30.276	1.00	37.97	N
ATOM	2928	C	HIS	B	423	14.525	34.142	31.341	1.00	37.06	C
ATOM	2929	O	HIS	B	423	13.989	35.236	31.153	1.00	39.39	O
ATOM	2930	N	LYS	B	424	13.927	33.149	31.995	1.00	28.98	N
ATOM	2931	CA	LYS	B	424	12.576	33.351	32.510	1.00	31.22	C
ATOM	2932	CB	LYS	B	424	11.957	32.006	32.883	1.00	28.63	C
ATOM	2933	CG	LYS	B	424	11.695	31.126	31.674	1.00	29.72	C
ATOM	2934	CD	LYS	B	424	11.076	29.800	32.117	1.00	42.69	C
ATOM	2935	CE	LYS	B	424	10.935	28.829	30.955	1.00	47.20	C
ATOM	2936	NZ	LYS	B	424	9.949	27.753	31.294	1.00	54.05	N
ATOM	2937	C	LYS	B	424	12.554	34.296	33.700	1.00	33.37	C
ATOM	2938	O	LYS	B	424	11.608	35.064	33.878	1.00	28.31	O
ATOM	2939	N	PHE	B	425	13.602	34.269	34.519	1.00	28.20	N
ATOM	2940	CA	PHE	B	425	13.660	35.137	35.681	1.00	26.95	C
ATOM	2941	CB	PHE	B	425	14.890	34.802	36.540	1.00	31.21	C
ATOM	2942	CG	PHE	B	425	15.042	35.680	37.747	1.00	32.76	C
ATOM	2943	CD1	PHE	B	425	14.318	35.431	38.904	1.00	41.67	C
ATOM	2944	CD2	PHE	B	425	15.886	36.782	37.710	1.00	35.66	C
ATOM	2945	CE1	PHE	B	425	14.429	36.272	40.011	1.00	40.79	C
ATOM	2946	CE2	PHE	B	425	16.010	37.631	38.805	1.00	43.64	C
ATOM	2947	CZ	PHE	B	425	15.277	37.377	39.962	1.00	45.58	C
ATOM	2948	C	PHE	B	425	13.713	36.629	35.310	1.00	28.99	C
ATOM	2949	O	PHE	B	425	13.149	37.468	36.010	1.00	28.02	O
ATOM	2950	N	LEU	B	426	14.379	36.961	34.212	1.00	27.54	N
ATOM	2951	CA	LEU	B	426	14.522	38.373	33.838	1.00	23.94	C
ATOM	2952	CB	LEU	B	426	15.838	38.577	33.072	1.00	25.46	C

ATOM	2953	CG	LEU	B	426	17.102	38.323	33.905	1.00	23.52	C
ATOM	2954	CD1	LEU	B	426	18.345	38.424	33.014	1.00	25.22	C
ATOM	2955	CD2	LEU	B	426	17.165	39.329	35.029	1.00	28.05	C
ATOM	2956	C	LEU	B	426	13.368	38.959	33.019	1.00	28.74	C
ATOM	2957	O	LEU	B	426	13.236	40.186	32.937	1.00	26.14	O
ATOM	2958	N	VAL	B	427	12.553	38.100	32.415	1.00	27.70	N
ATOM	2959	CA	VAL	B	427	11.442	38.584	31.583	1.00	30.96	C
ATOM	2960	CB	VAL	B	427	10.577	37.409	31.059	1.00	35.17	C
ATOM	2961	CG1	VAL	B	427	9.323	37.939	30.343	1.00	34.67	C
ATOM	2962	CG2	VAL	B	427	11.391	36.561	30.082	1.00	31.17	C
ATOM	2963	C	VAL	B	427	10.551	39.581	32.331	1.00	36.19	C
ATOM	2964	O	VAL	B	427	9.984	39.269	33.386	1.00	37.99	O
ATOM	2965	N	GLY	B	428	10.454	40.791	31.788	1.00	44.92	N
ATOM	2966	CA	GLY	B	428	9.637	41.830	32.397	1.00	39.36	C
ATOM	2967	C	GLY	B	428	10.144	42.432	33.696	1.00	46.68	C
ATOM	2968	O	GLY	B	428	9.384	43.091	34.410	1.00	43.86	O
ATOM	2969	N	LYS	B	429	11.419	42.231	34.019	1.00	36.36	N
ATOM	2970	CA	LYS	B	429	11.960	42.772	35.258	1.00	41.33	C
ATOM	2971	CB	LYS	B	429	12.561	41.638	36.086	1.00	45.43	C
ATOM	2972	CG	LYS	B	429	11.519	40.599	36.492	1.00	48.96	C
ATOM	2973	CD	LYS	B	429	11.975	39.804	37.699	1.00	53.23	C
ATOM	2974	CE	LYS	B	429	11.004	38.680	38.025	1.00	52.24	C
ATOM	2975	NZ	LYS	B	429	11.552	37.819	39.108	1.00	60.84	N
ATOM	2976	C	LYS	B	429	12.990	43.880	35.028	1.00	42.92	C
ATOM	2977	O	LYS	B	429	13.841	44.152	35.883	1.00	41.32	O
ATOM	2978	N	ARG	B	430	12.889	44.535	33.878	1.00	38.04	N
ATOM	2979	CA	ARG	B	430	13.824	45.594	33.532	1.00	50.47	C
ATOM	2980	CB	ARG	B	430	13.541	46.091	32.116	1.00	52.47	C
ATOM	2981	CG	ARG	B	430	14.669	46.918	31.520	1.00	63.31	C
ATOM	2982	CD	ARG	B	430	14.548	47.014	29.999	1.00	63.30	C
ATOM	2983	NE	ARG	B	430	15.857	46.896	29.351	1.00	63.29	N
ATOM	2984	CZ	ARG	B	430	16.061	46.254	28.203	1.00	68.48	C
ATOM	2985	NH1	ARG	B	430	15.043	45.680	27.573	1.00	63.45	N
ATOM	2986	NH2	ARG	B	430	17.294	46.151	27.698	1.00	66.07	N
ATOM	2987	C	ARG	B	430	13.774	46.754	34.518	1.00	53.77	C
ATOM	2988	O	ARG	B	430	14.727	47.516	34.643	1.00	53.09	O
ATOM	2989	N	GLU	B	431	12.661	46.879	35.235	1.00	54.55	N
ATOM	2990	CA	GLU	B	431	12.518	47.959	36.196	1.00	55.49	C
ATOM	2991	CB	GLU	B	431	11.167	48.658	36.020	1.00	57.64	C
ATOM	2992	CG	GLU	B	431	11.104	49.556	34.797	1.00	61.36	C
ATOM	2993	CD	GLU	B	431	9.932	50.515	34.839	1.00	66.74	C
ATOM	2994	OE1	GLU	B	431	9.882	51.356	35.767	1.00	71.47	O
ATOM	2995	OE2	GLU	B	431	9.062	50.433	33.946	1.00	68.60	O
ATOM	2996	C	GLU	B	431	12.683	47.510	37.635	1.00	56.39	C
ATOM	2997	O	GLU	B	431	12.608	48.325	38.550	1.00	57.92	O
ATOM	2998	N	GLU	B	432	12.910	46.218	37.844	1.00	51.06	N
ATOM	2999	CA	GLU	B	432	13.091	45.720	39.194	1.00	50.31	C
ATOM	3000	CB	GLU	B	432	11.992	44.713	39.554	1.00	56.46	C
ATOM	3001	CG	GLU	B	432	12.301	43.274	39.217	1.00	60.14	C
ATOM	3002	CD	GLU	B	432	11.319	42.313	39.866	1.00	63.83	C
ATOM	3003	OE1	GLU	B	432	10.118	42.375	39.526	1.00	66.40	O
ATOM	3004	OE2	GLU	B	432	11.746	41.501	40.719	1.00	66.50	O
ATOM	3005	C	GLU	B	432	14.464	45.083	39.364	1.00	49.21	C
ATOM	3006	O	GLU	B	432	14.932	44.892	40.483	1.00	47.48	O
ATOM	3007	N	ILE	B	433	15.111	44.756	38.246	1.00	43.34	N
ATOM	3008	CA	ILE	B	433	16.442	44.156	38.288	1.00	35.43	C
ATOM	3009	CB	ILE	B	433	16.436	42.734	37.688	1.00	40.48	C
ATOM	3010	CG2	ILE	B	433	17.842	42.125	37.754	1.00	33.02	C
ATOM	3011	CG1	ILE	B	433	15.463	41.850	38.460	1.00	39.44	C
ATOM	3012	CD1	ILE	B	433	15.862	41.633	39.896	1.00	42.99	C
ATOM	3013	C	ILE	B	433	17.335	45.049	37.446	1.00	37.58	C
ATOM	3014	O	ILE	B	433	17.309	44.975	36.217	1.00	33.88	O
ATOM	3015	N	PRO	B	434	18.125	45.919	38.097	1.00	33.22	N
ATOM	3016	CD	PRO	B	434	18.093	46.179	39.546	1.00	39.68	C
ATOM	3017	CA	PRO	B	434	19.038	46.857	37.435	1.00	37.36	C
ATOM	3018	CB	PRO	B	434	19.661	47.606	38.614	1.00	36.58	C
ATOM	3019	CG	PRO	B	434	18.559	47.616	39.604	1.00	47.33	C
ATOM	3020	C	PRO	B	434	20.083	46.163	36.578	1.00	35.02	C

ATOM	3021	O	PRO	B	434	20.382	44.986	36.785	1.00 29.87	O
ATOM	3022	N	VAL	B	435	20.644	46.904	35.625	1.00 30.90	N
ATOM	3023	CA	VAL	B	435	21.669	46.349	34.750	1.00 33.32	C
ATOM	3024	CB	VAL	B	435	22.138	47.391	33.699	1.00 32.31	C
ATOM	3025	CG1	VAL	B	435	23.255	46.802	32.839	1.00 32.23	C
ATOM	3026	CG2	VAL	B	435	20.968	47.792	32.821	1.00 38.32	C
ATOM	3027	C	VAL	B	435	22.862	45.875	35.570	1.00 31.88	C
ATOM	3028	O	VAL	B	435	23.504	44.873	35.218	1.00 26.54	O
ATOM	3029	N	SER	B	436	23.165	46.593	36.652	1.00 28.96	N
ATOM	3030	CA	SER	B	436	24.278	46.225	37.519	1.00 29.85	C
ATOM	3031	CB	SER	B	436	24.437	47.262	38.646	1.00 33.71	C
ATOM	3032	OG	SER	B	436	23.246	47.361	39.414	1.00 36.37	O
ATOM	3033	C	SER	B	436	24.077	44.815	38.112	1.00 30.64	C
ATOM	3034	O	SER	B	436	25.039	44.069	38.281	1.00 28.51	O
ATOM	3035	N	ASN	B	437	22.832	44.464	38.426	1.00 25.41	N
ATOM	3036	CA	ASN	B	437	22.502	43.155	38.993	1.00 26.86	C
ATOM	3037	CB	ASN	B	437	21.088	43.219	39.581	1.00 29.47	C
ATOM	3038	CG	ASN	B	437	20.692	41.975	40.391	1.00 32.65	C
ATOM	3039	OD1	ASN	B	437	19.669	41.997	41.081	1.00 33.91	O
ATOM	3040	ND2	ASN	B	437	21.466	40.891	40.294	1.00 29.62	N
ATOM	3041	C	ASN	B	437	22.632	42.121	37.858	1.00 26.75	C
ATOM	3042	O	ASN	B	437	23.126	41.010	38.070	1.00 26.10	O
ATOM	3043	N	VAL	B	438	22.220	42.483	36.648	1.00 26.29	N
ATOM	3044	CA	VAL	B	438	22.390	41.546	35.548	1.00 22.79	C
ATOM	3045	CB	VAL	B	438	21.761	42.073	34.250	1.00 26.63	C
ATOM	3046	CG1	VAL	B	438	22.085	41.136	33.099	1.00 25.60	C
ATOM	3047	CG2	VAL	B	438	20.231	42.187	34.428	1.00 27.00	C
ATOM	3048	C	VAL	B	438	23.896	41.313	35.343	1.00 25.06	C
ATOM	3049	O	VAL	B	438	24.325	40.178	35.172	1.00 22.07	O
ATOM	3050	N	ALA	B	439	24.704	42.383	35.376	1.00 23.57	N
ATOM	3051	CA	ALA	B	439	26.156	42.223	35.206	1.00 24.57	C
ATOM	3052	CB	ALA	B	439	26.858	43.623	35.135	1.00 23.14	C
ATOM	3053	C	ALA	B	439	26.775	41.369	36.326	1.00 21.99	C
ATOM	3054	O	ALA	B	439	27.724	40.622	36.086	1.00 23.36	O
ATOM	3055	N	GLU	B	440	26.225	41.467	37.540	1.00 22.47	N
ATOM	3056	CA	GLU	B	440	26.729	40.684	38.660	1.00 26.63	C
ATOM	3057	CB	GLU	B	440	25.946	41.027	39.937	1.00 28.89	C
ATOM	3058	CG	GLU	B	440	26.220	40.080	41.109	1.00 27.35	C
ATOM	3059	CD	GLU	B	440	25.304	40.355	42.295	1.00 39.88	C
ATOM	3060	OE1	GLU	B	440	24.142	40.766	42.075	1.00 37.76	O
ATOM	3061	OE2	GLU	B	440	25.750	40.145	43.445	1.00 37.86	O
ATOM	3062	C	GLU	B	440	26.575	39.190	38.331	1.00 28.92	C
ATOM	3063	O	GLU	B	440	27.503	38.411	38.506	1.00 22.24	O
ATOM	3064	N	LEU	B	441	25.393	38.812	37.848	1.00 22.17	N
ATOM	3065	CA	LEU	B	441	25.086	37.423	37.488	1.00 22.51	C
ATOM	3066	CB	LEU	B	441	23.590	37.301	37.148	1.00 22.22	C
ATOM	3067	CG	LEU	B	441	22.647	37.692	38.290	1.00 26.11	C
ATOM	3068	CD1	LEU	B	441	21.191	37.675	37.823	1.00 26.08	C
ATOM	3069	CD2	LEU	B	441	22.853	36.702	39.443	1.00 23.20	C
ATOM	3070	C	LEU	B	441	25.930	36.973	36.296	1.00 20.83	C
ATOM	3071	O	LEU	B	441	26.449	35.848	36.280	1.00 22.40	O
ATOM	3072	N	LEU	B	442	26.062	37.829	35.290	1.00 20.51	N
ATOM	3073	CA	LEU	B	442	26.893	37.442	34.147	1.00 24.46	C
ATOM	3074	CB	LEU	B	442	26.822	38.487	33.038	1.00 22.94	C
ATOM	3075	CG	LEU	B	442	25.484	38.527	32.291	1.00 21.56	C
ATOM	3076	CD1	LEU	B	442	25.459	39.693	31.263	1.00 24.52	C
ATOM	3077	CD2	LEU	B	442	25.268	37.168	31.601	1.00 22.91	C
ATOM	3078	C	LEU	B	442	28.346	37.244	34.590	1.00 21.94	C
ATOM	3079	O	LEU	B	442	29.033	36.352	34.105	1.00 22.31	O
ATOM	3080	N	HIS	B	443	28.811	38.055	35.530	1.00 20.83	N
ATOM	3081	CA	HIS	B	443	30.193	37.888	35.998	1.00 21.14	C
ATOM	3082	CB	HIS	B	443	30.598	39.048	36.918	1.00 25.52	C
ATOM	3083	CG	HIS	B	443	31.965	38.875	37.502	1.00 27.68	C
ATOM	3084	CD2	HIS	B	443	33.143	38.507	36.932	1.00 25.68	C
ATOM	3085	ND1	HIS	B	443	32.210	38.987	38.855	1.00 26.29	N
ATOM	3086	CE1	HIS	B	443	33.476	38.691	39.096	1.00 24.28	C
ATOM	3087	NE2	HIS	B	443	34.064	38.394	37.947	1.00 23.65	N
ATOM	3088	C	HIS	B	443	30.367	36.530	36.715	1.00 22.96	C

ATOM	3089	O	HIS	B	443	31.374	35.841	36.541	1.00	21.47	O
ATOM	3090	N	GLN	B	444	29.370	36.130	37.498	1.00	22.87	N
ATOM	3091	CA	GLN	B	444	29.429	34.843	38.177	1.00	19.38	C
ATOM	3092	CB	GLN	B	444	28.203	34.688	39.080	1.00	21.91	C
ATOM	3093	CG	GLN	B	444	28.254	35.697	40.221	1.00	22.66	C
ATOM	3094	CD	GLN	B	444	27.013	35.648	41.058	1.00	25.66	C
ATOM	3095	OE1	GLN	B	444	25.994	35.130	40.633	1.00	27.50	O
ATOM	3096	NE2	GLN	B	444	27.089	36.206	42.258	1.00	27.58	N
ATOM	3097	C	GLN	B	444	29.483	33.735	37.149	1.00	22.05	C
ATOM	3098	O	GLN	B	444	30.248	32.792	37.288	1.00	23.64	O
ATOM	3099	N	VAL	B	445	28.691	33.867	36.089	1.00	20.47	N
ATOM	3100	CA	VAL	B	445	28.735	32.863	35.044	1.00	19.55	C
ATOM	3101	CB	VAL	B	445	27.705	33.147	33.926	1.00	20.65	C
ATOM	3102	CG1	VAL	B	445	27.876	32.121	32.784	1.00	21.65	C
ATOM	3103	CG2	VAL	B	445	26.300	33.049	34.493	1.00	21.06	C
ATOM	3104	C	VAL	B	445	30.151	32.857	34.435	1.00	21.63	C
ATOM	3105	O	VAL	B	445	30.682	31.792	34.150	1.00	21.53	O
ATOM	3106	N	SER	B	446	30.757	34.031	34.251	1.00	19.30	N
ATOM	3107	CA	SER	B	446	32.108	34.047	33.663	1.00	22.00	C
ATOM	3108	CB	SER	B	446	32.570	35.480	33.292	1.00	19.55	C
ATOM	3109	OG	SER	B	446	32.902	36.261	34.407	1.00	22.80	O
ATOM	3110	C	SER	B	446	33.142	33.399	34.600	1.00	22.37	C
ATOM	3111	O	SER	B	446	34.109	32.812	34.131	1.00	21.37	O
ATOM	3112	N	MET	B	447	32.925	33.497	35.909	1.00	20.23	N
ATOM	3113	CA	MET	B	447	33.860	32.859	36.846	1.00	24.29	C
ATOM	3114	CB	MET	B	447	33.640	33.376	38.272	1.00	23.41	C
ATOM	3115	CG	MET	B	447	34.123	34.806	38.446	1.00	27.21	C
ATOM	3116	SD	MET	B	447	34.087	35.327	40.218	1.00	29.84	S
ATOM	3117	CE	MET	B	447	32.347	35.711	40.421	1.00	28.71	C
ATOM	3118	C	MET	B	447	33.698	31.342	36.767	1.00	24.03	C
ATOM	3119	O	MET	B	447	34.681	30.617	36.778	1.00	23.04	O
ATOM	3120	N	GLY	B	448	32.460	30.858	36.669	1.00	19.35	N
ATOM	3121	CA	GLY	B	448	32.276	29.423	36.546	1.00	21.93	C
ATOM	3122	C	GLY	B	448	32.898	28.922	35.248	1.00	28.63	C
ATOM	3123	O	GLY	B	448	33.506	27.847	35.242	1.00	23.12	O
ATOM	3124	N	MET	B	449	32.758	29.687	34.155	1.00	21.69	N
ATOM	3125	CA	MET	B	449	33.325	29.240	32.866	1.00	20.45	C
ATOM	3126	CB	MET	B	449	32.714	30.027	31.692	1.00	22.80	C
ATOM	3127	CG	MET	B	449	31.201	29.789	31.468	1.00	21.04	C
ATOM	3128	SD	MET	B	449	30.734	28.035	31.300	1.00	25.98	S
ATOM	3129	CE	MET	B	449	31.656	27.593	29.836	1.00	24.75	C
ATOM	3130	C	MET	B	449	34.852	29.343	32.825	1.00	19.20	C
ATOM	3131	O	MET	B	449	35.526	28.532	32.182	1.00	23.26	O
ATOM	3132	N	LYS	B	450	35.399	30.330	33.520	1.00	21.31	N
ATOM	3133	CA	LYS	B	450	36.847	30.477	33.578	1.00	22.27	C
ATOM	3134	CB	LYS	B	450	37.188	31.710	34.397	1.00	25.65	C
ATOM	3135	CG	LYS	B	450	38.686	31.870	34.602	1.00	35.16	C
ATOM	3136	CD	LYS	B	450	38.967	32.940	35.604	1.00	39.35	C
ATOM	3137	CE	LYS	B	450	40.432	32.855	36.005	1.00	41.39	C
ATOM	3138	NZ	LYS	B	450	40.770	33.998	36.884	1.00	50.53	N
ATOM	3139	C	LYS	B	450	37.382	29.201	34.259	1.00	21.58	C
ATOM	3140	O	LYS	B	450	38.394	28.634	33.863	1.00	23.54	O
ATOM	3141	N	TYR	B	451	36.667	28.738	35.272	1.00	22.85	N
ATOM	3142	CA	TYR	B	451	37.061	27.508	35.980	1.00	26.56	C
ATOM	3143	CB	TYR	B	451	36.179	27.307	37.225	1.00	31.08	C
ATOM	3144	CG	TYR	B	451	36.420	25.996	37.963	1.00	26.37	C
ATOM	3145	CD1	TYR	B	451	37.523	25.831	38.813	1.00	32.42	C
ATOM	3146	CE1	TYR	B	451	37.719	24.612	39.503	1.00	35.50	C
ATOM	3147	CD2	TYR	B	451	35.543	24.934	37.810	1.00	29.25	C
ATOM	3148	CE2	TYR	B	451	35.737	23.731	38.458	1.00	36.41	C
ATOM	3149	CZ	TYR	B	451	36.814	23.570	39.307	1.00	36.89	C
ATOM	3150	OH	TYR	B	451	36.928	22.357	39.947	1.00	35.03	O
ATOM	3151	C	TYR	B	451	36.975	26.290	35.084	1.00	23.27	C
ATOM	3152	O	TYR	B	451	37.904	25.484	35.035	1.00	22.89	O
ATOM	3153	N	LEU	B	452	35.881	26.144	34.339	1.00	21.39	N
ATOM	3154	CA	LEU	B	452	35.757	25.005	33.457	1.00	21.19	C
ATOM	3155	CB	LEU	B	452	34.379	24.995	32.735	1.00	25.34	C
ATOM	3156	CG	LEU	B	452	33.197	24.695	33.653	1.00	31.38	C

ATOM	3157	CD1	LEU	B	452	31.922	24.872	32.832	1.00	39.34	C
ATOM	3158	CD2	LEU	B	452	33.275	23.271	34.196	1.00	34.35	C
ATOM	3159	C	LEU	B	452	36.855	24.995	32.417	1.00	23.04	C
ATOM	3160	O	LEU	B	452	37.399	23.930	32.098	1.00	23.98	O
ATOM	3161	N	GLU	B	453	37.178	26.179	31.894	1.00	21.93	N
ATOM	3162	CA	GLU	B	453	38.215	26.298	30.881	1.00	24.62	C
ATOM	3163	CB	GLU	B	453	38.283	27.747	30.398	1.00	25.46	C
ATOM	3164	CG	GLU	B	453	39.415	28.050	29.406	1.00	28.82	C
ATOM	3165	CD	GLU	B	453	39.405	29.510	28.934	1.00	36.37	C
ATOM	3166	OE1	GLU	B	453	40.016	30.376	29.621	1.00	33.79	O
ATOM	3167	OE2	GLU	B	453	38.776	29.790	27.880	1.00	31.16	O
ATOM	3168	C	GLU	B	453	39.585	25.865	31.454	1.00	25.13	C
ATOM	3169	O	GLU	B	453	40.345	25.115	30.812	1.00	25.39	O
ATOM	3170	N	GLU	B	454	39.908	26.351	32.645	1.00	22.62	N
ATOM	3171	CA	GLU	B	454	41.204	25.996	33.245	1.00	26.22	C
ATOM	3172	CB	GLU	B	454	41.436	26.762	34.552	1.00	30.29	C
ATOM	3173	CG	GLU	B	454	40.519	26.379	35.681	1.00	43.54	C
ATOM	3174	CD	GLU	B	454	40.821	27.144	36.972	1.00	58.22	C
ATOM	3175	OE1	GLU	B	454	40.838	28.404	36.941	1.00	50.28	O
ATOM	3176	OE2	GLU	B	454	41.029	26.480	38.019	1.00	56.54	O
ATOM	3177	C	GLU	B	454	41.284	24.501	33.507	1.00	32.56	C
ATOM	3178	O	GLU	B	454	42.368	23.927	33.489	1.00	31.49	O
ATOM	3179	N	LYS	B	455	40.147	23.852	33.728	1.00	26.00	N
ATOM	3180	CA	LYS	B	455	40.141	22.406	33.979	1.00	27.14	C
ATOM	3181	CB	LYS	B	455	39.043	22.032	34.991	1.00	26.60	C
ATOM	3182	CG	LYS	B	455	39.173	22.743	36.346	1.00	29.96	C
ATOM	3183	CD	LYS	B	455	40.493	22.365	37.009	1.00	36.01	C
ATOM	3184	CE	LYS	B	455	40.733	23.118	38.322	1.00	40.11	C
ATOM	3185	NZ	LYS	B	455	42.067	22.747	38.909	1.00	33.10	N
ATOM	3186	C	LYS	B	455	39.954	21.605	32.692	1.00	26.89	C
ATOM	3187	O	LYS	B	455	39.757	20.397	32.732	1.00	31.85	O
ATOM	3188	N	ASN	B	456	40.047	22.280	31.551	1.00	27.82	N
ATOM	3189	CA	ASN	B	456	39.901	21.640	30.245	1.00	30.31	C
ATOM	3190	CB	ASN	B	456	41.089	20.707	29.967	1.00	32.92	C
ATOM	3191	CG	ASN	B	456	42.384	21.456	29.907	1.00	40.95	C
ATOM	3192	OD1	ASN	B	456	42.556	22.351	29.081	1.00	37.33	O
ATOM	3193	ND2	ASN	B	456	43.313	21.110	30.803	1.00	43.15	N
ATOM	3194	C	ASN	B	456	38.602	20.891	29.992	1.00	30.21	C
ATOM	3195	O	ASN	B	456	38.614	19.772	29.473	1.00	28.50	O
ATOM	3196	N	PHE	B	457	37.482	21.494	30.381	1.00	25.11	N
ATOM	3197	CA	PHE	B	457	36.193	20.899	30.098	1.00	22.51	C
ATOM	3198	CB	PHE	B	457	35.376	20.679	31.386	1.00	23.31	C
ATOM	3199	CG	PHE	B	457	35.848	19.515	32.204	1.00	26.75	C
ATOM	3200	CD1	PHE	B	457	36.692	19.706	33.302	1.00	38.60	C
ATOM	3201	CD2	PHE	B	457	35.456	18.232	31.877	1.00	29.58	C
ATOM	3202	CE1	PHE	B	457	37.125	18.614	34.055	1.00	40.07	C
ATOM	3203	CE2	PHE	B	457	35.887	17.140	32.624	1.00	35.33	C
ATOM	3204	CZ	PHE	B	457	36.718	17.334	33.710	1.00	29.78	C
ATOM	3205	C	PHE	B	457	35.435	21.903	29.198	1.00	20.08	C
ATOM	3206	O	PHE	B	457	35.555	23.105	29.396	1.00	24.84	O
ATOM	3207	N	VAL	B	458	34.657	21.370	28.247	1.00	22.46	N
ATOM	3208	CA	VAL	B	458	33.832	22.189	27.351	1.00	19.50	C
ATOM	3209	CB	VAL	B	458	34.039	21.771	25.864	1.00	24.51	C
ATOM	3210	CG1	VAL	B	458	33.044	22.521	24.946	1.00	20.39	C
ATOM	3211	CG2	VAL	B	458	35.451	22.094	25.438	1.00	26.69	C
ATOM	3212	C	VAL	B	458	32.365	21.908	27.749	1.00	22.31	C
ATOM	3213	O	VAL	B	458	31.956	20.779	27.818	1.00	23.69	O
ATOM	3214	N	HIS	B	459	31.581	22.946	27.977	1.00	21.21	N
ATOM	3215	CA	HIS	B	459	30.176	22.720	28.415	1.00	20.87	C
ATOM	3216	CB	HIS	B	459	29.670	23.998	29.119	1.00	26.99	C
ATOM	3217	CG	HIS	B	459	28.294	23.866	29.693	1.00	26.79	C
ATOM	3218	CD2	HIS	B	459	27.869	23.814	30.978	1.00	33.82	C
ATOM	3219	ND1	HIS	B	459	27.163	23.762	28.912	1.00	30.62	N
ATOM	3220	CE1	HIS	B	459	26.099	23.665	29.691	1.00	28.63	C
ATOM	3221	NE2	HIS	B	459	26.500	23.693	30.949	1.00	26.47	N
ATOM	3222	C	HIS	B	459	29.279	22.376	27.225	1.00	22.74	C
ATOM	3223	O	HIS	B	459	28.472	21.409	27.260	1.00	26.21	O
ATOM	3224	N	ARG	B	460	29.432	23.186	26.178	1.00	23.74	N

ATOM	3225	CA	ARG	B	460	28.716	23.083	24.911	1.00	23.96	C
ATOM	3226	CB	ARG	B	460	28.766	21.644	24.390	1.00	27.31	C
ATOM	3227	CG	ARG	B	460	28.259	21.546	22.972	1.00	37.56	C
ATOM	3228	CD	ARG	B	460	28.279	20.147	22.427	1.00	32.14	C
ATOM	3229	NE	ARG	B	460	27.254	20.032	21.406	1.00	31.71	N
ATOM	3230	CZ	ARG	B	460	27.008	18.927	20.699	1.00	39.03	C
ATOM	3231	NH1	ARG	B	460	27.721	17.830	20.903	1.00	34.17	N
ATOM	3232	NH2	ARG	B	460	26.040	18.924	19.793	1.00	42.19	N
ATOM	3233	C	ARG	B	460	27.261	23.562	24.895	1.00	30.30	C
ATOM	3234	O	ARG	B	460	26.726	23.888	23.833	1.00	37.44	O
ATOM	3235	N	ASP	B	461	26.628	23.648	26.054	1.00	24.84	N
ATOM	3236	CA	ASP	B	461	25.230	24.057	26.087	1.00	27.22	C
ATOM	3237	CB	ASP	B	461	24.389	22.843	26.547	1.00	29.93	C
ATOM	3238	CG	ASP	B	461	22.893	22.954	26.185	1.00	40.58	C
ATOM	3239	OD1	ASP	B	461	22.497	23.822	25.374	1.00	47.29	O
ATOM	3240	OD2	ASP	B	461	22.100	22.138	26.718	1.00	51.22	O
ATOM	3241	C	ASP	B	461	25.039	25.281	26.998	1.00	27.48	C
ATOM	3242	O	ASP	B	461	24.054	25.401	27.713	1.00	25.86	O
ATOM	3243	N	LEU	B	462	25.985	26.210	26.963	1.00	21.15	N
ATOM	3244	CA	LEU	B	462	25.841	27.399	27.788	1.00	20.41	C
ATOM	3245	CB	LEU	B	462	27.200	28.106	27.940	1.00	22.91	C
ATOM	3246	CG	LEU	B	462	27.216	29.380	28.792	1.00	28.71	C
ATOM	3247	CD1	LEU	B	462	26.774	29.008	30.203	1.00	30.96	C
ATOM	3248	CD2	LEU	B	462	28.614	30.037	28.792	1.00	27.89	C
ATOM	3249	C	LEU	B	462	24.790	28.300	27.113	1.00	25.32	C
ATOM	3250	O	LEU	B	462	24.913	28.640	25.958	1.00	27.45	O
ATOM	3251	N	ALA	B	463	23.737	28.637	27.847	1.00	20.92	N
ATOM	3252	CA	ALA	B	463	22.645	29.482	27.350	1.00	20.29	C
ATOM	3253	CB	ALA	B	463	21.709	28.658	26.431	1.00	17.73	C
ATOM	3254	C	ALA	B	463	21.905	29.962	28.596	1.00	21.81	C
ATOM	3255	O	ALA	B	463	21.978	29.319	29.655	1.00	21.64	O
ATOM	3256	N	ALA	B	464	21.187	31.069	28.492	1.00	19.40	N
ATOM	3257	CA	ALA	B	464	20.510	31.586	29.655	1.00	21.46	C
ATOM	3258	CB	ALA	B	464	19.750	32.879	29.294	1.00	20.54	C
ATOM	3259	C	ALA	B	464	19.567	30.560	30.288	1.00	23.11	C
ATOM	3260	O	ALA	B	464	19.399	30.567	31.499	1.00	22.21	O
ATOM	3261	N	ARG	B	465	18.963	29.703	29.468	1.00	22.19	N
ATOM	3262	CA	ARG	B	465	18.036	28.679	29.955	1.00	25.34	C
ATOM	3263	CB	ARG	B	465	17.372	27.947	28.783	1.00	22.79	C
ATOM	3264	CG	ARG	B	465	18.310	27.131	27.897	1.00	21.09	C
ATOM	3265	CD	ARG	B	465	17.586	26.576	26.650	1.00	28.36	C
ATOM	3266	NE	ARG	B	465	18.537	25.936	25.752	1.00	33.20	N
ATOM	3267	CZ	ARG	B	465	19.230	26.568	24.801	1.00	41.11	C
ATOM	3268	NH1	ARG	B	465	19.074	27.873	24.592	1.00	34.56	N
ATOM	3269	NH2	ARG	B	465	20.129	25.908	24.099	1.00	36.89	N
ATOM	3270	C	ARG	B	465	18.746	27.650	30.840	1.00	27.21	C
ATOM	3271	O	ARG	B	465	18.098	26.930	31.600	1.00	25.31	O
ATOM	3272	N	ASN	B	466	20.075	27.583	30.727	1.00	26.22	N
ATOM	3273	CA	ASN	B	466	20.851	26.640	31.535	1.00	22.74	C
ATOM	3274	CB	ASN	B	466	21.777	25.809	30.647	1.00	20.44	C
ATOM	3275	CG	ASN	B	466	21.022	24.810	29.806	1.00	31.49	C
ATOM	3276	OD1	ASN	B	466	19.963	24.316	30.217	1.00	26.09	O
ATOM	3277	ND2	ASN	B	466	21.556	24.496	28.624	1.00	25.81	N
ATOM	3278	C	ASN	B	466	21.608	27.277	32.677	1.00	24.14	C
ATOM	3279	O	ASN	B	466	22.379	26.617	33.372	1.00	25.61	O
ATOM	3280	N	VAL	B	467	21.384	28.563	32.895	1.00	19.90	N
ATOM	3281	CA	VAL	B	467	21.999	29.239	34.013	1.00	18.65	C
ATOM	3282	CB	VAL	B	467	22.443	30.652	33.640	1.00	21.94	C
ATOM	3283	CG1	VAL	B	467	22.840	31.414	34.910	1.00	20.29	C
ATOM	3284	CG2	VAL	B	467	23.617	30.565	32.634	1.00	21.43	C
ATOM	3285	C	VAL	B	467	20.834	29.323	35.002	1.00	25.03	C
ATOM	3286	O	VAL	B	467	19.757	29.829	34.659	1.00	24.55	O
ATOM	3287	N	LEU	B	468	21.047	28.821	36.212	1.00	21.56	N
ATOM	3288	CA	LEU	B	468	19.972	28.813	37.219	1.00	22.81	C
ATOM	3289	CB	LEU	B	468	19.738	27.385	37.734	1.00	22.41	C
ATOM	3290	CG	LEU	B	468	19.493	26.291	36.695	1.00	25.80	C
ATOM	3291	CD1	LEU	B	468	19.568	24.927	37.347	1.00	27.13	C
ATOM	3292	CD2	LEU	B	468	18.128	26.521	36.038	1.00	28.96	C

ATOM	3293	C	LEU	B	468	20.287	29.707	38.394	1.00	27.22	C
ATOM	3294	O	LEU	B	468	21.426	29.782	38.826	1.00	26.70	O
ATOM	3295	N	LEU	B	469	19.262	30.349	38.960	1.00	24.32	N
ATOM	3296	CA	LEU	B	469	19.511	31.234	40.078	1.00	23.08	C
ATOM	3297	CB	LEU	B	469	18.687	32.498	39.908	1.00	24.42	C
ATOM	3298	CG	LEU	B	469	18.985	33.232	38.596	1.00	37.62	C
ATOM	3299	CD1	LEU	B	469	17.999	34.336	38.412	1.00	40.80	C
ATOM	3300	CD2	LEU	B	469	20.384	33.797	38.612	1.00	33.91	C
ATOM	3301	C	LEU	B	469	19.216	30.625	41.440	1.00	26.89	C
ATOM	3302	O	LEU	B	469	18.162	30.024	41.643	1.00	27.22	O
ATOM	3303	N	VAL	B	470	20.154	30.766	42.366	1.00	27.63	N
ATOM	3304	CA	VAL	B	470	19.903	30.311	43.718	1.00	30.31	C
ATOM	3305	CB	VAL	B	470	21.199	30.132	44.520	1.00	33.68	C
ATOM	3306	CG1	VAL	B	470	20.862	29.797	45.973	1.00	34.34	C
ATOM	3307	CG2	VAL	B	470	22.027	29.002	43.912	1.00	28.72	C
ATOM	3308	C	VAL	B	470	19.057	31.450	44.300	1.00	31.84	C
ATOM	3309	O	VAL	B	470	18.096	31.210	45.051	1.00	33.69	O
ATOM	3310	N	ASN	B	471	19.407	32.682	43.930	1.00	29.94	N
ATOM	3311	CA	ASN	B	471	18.688	33.903	44.335	1.00	34.01	C
ATOM	3312	CB	ASN	B	471	19.139	34.394	45.723	1.00	38.51	C
ATOM	3313	CG	ASN	B	471	20.631	34.554	45.824	1.00	41.61	C
ATOM	3314	OD1	ASN	B	471	21.336	33.627	46.225	1.00	62.13	O
ATOM	3315	ND2	ASN	B	471	21.129	35.710	45.433	1.00	34.16	N
ATOM	3316	C	ASN	B	471	19.009	34.971	43.283	1.00	32.05	C
ATOM	3317	O	ASN	B	471	19.796	34.712	42.378	1.00	29.59	O
ATOM	3318	N	ARG	B	472	18.434	36.170	43.395	1.00	31.13	N
ATOM	3319	CA	ARG	B	472	18.687	37.216	42.392	1.00	33.64	C
ATOM	3320	CB	ARG	B	472	17.766	38.417	42.631	1.00	35.84	C
ATOM	3321	CG	ARG	B	472	18.042	39.147	43.924	1.00	37.87	C
ATOM	3322	CD	ARG	B	472	17.142	40.371	44.053	1.00	40.99	C
ATOM	3323	NE	ARG	B	472	17.621	41.483	43.240	1.00	43.11	N
ATOM	3324	CZ	ARG	B	472	16.972	42.633	43.074	1.00	48.70	C
ATOM	3325	NH1	ARG	B	472	15.795	42.832	43.667	1.00	41.99	N
ATOM	3326	NH2	ARG	B	472	17.503	43.593	42.334	1.00	44.48	N
ATOM	3327	C	ARG	B	472	20.132	37.702	42.324	1.00	24.49	C
ATOM	3328	O	ARG	B	472	20.492	38.446	41.423	1.00	30.50	O
ATOM	3329	N	HIS	B	473	20.952	37.294	43.288	1.00	26.54	N
ATOM	3330	CA	HIS	B	473	22.340	37.700	43.324	1.00	30.93	C
ATOM	3331	CB	HIS	B	473	22.628	38.517	44.614	1.00	28.14	C
ATOM	3332	CG	HIS	B	473	21.888	39.817	44.673	1.00	32.49	C
ATOM	3333	CD2	HIS	B	473	20.856	40.225	45.451	1.00	40.34	C
ATOM	3334	ND1	HIS	B	473	22.125	40.845	43.786	1.00	36.03	N
ATOM	3335	CE1	HIS	B	473	21.266	41.825	44.008	1.00	41.10	C
ATOM	3336	NE2	HIS	B	473	20.482	41.473	45.013	1.00	42.57	N
ATOM	3337	C	HIS	B	473	23.276	36.497	43.260	1.00	25.86	C
ATOM	3338	O	HIS	B	473	24.472	36.628	43.573	1.00	25.18	O
ATOM	3339	N	TYR	B	474	22.760	35.337	42.854	1.00	26.93	N
ATOM	3340	CA	TYR	B	474	23.614	34.141	42.810	1.00	28.61	C
ATOM	3341	CB	TYR	B	474	23.597	33.447	44.184	1.00	26.00	C
ATOM	3342	CG	TYR	B	474	24.589	32.302	44.396	1.00	29.87	C
ATOM	3343	CD1	TYR	B	474	25.645	32.050	43.505	1.00	27.42	C
ATOM	3344	CE1	TYR	B	474	26.563	30.995	43.747	1.00	31.28	C
ATOM	3345	CD2	TYR	B	474	24.477	31.481	45.523	1.00	34.24	C
ATOM	3346	CE2	TYR	B	474	25.377	30.444	45.768	1.00	37.06	C
ATOM	3347	CZ	TYR	B	474	26.416	30.198	44.888	1.00	35.99	C
ATOM	3348	OH	TYR	B	474	27.285	29.160	45.187	1.00	32.29	O
ATOM	3349	C	TYR	B	474	23.218	33.160	41.719	1.00	27.49	C
ATOM	3350	O	TYR	B	474	22.237	32.413	41.862	1.00	27.72	O
ATOM	3351	N	ALA	B	475	24.003	33.153	40.638	1.00	21.66	N
ATOM	3352	CA	ALA	B	475	23.744	32.279	39.509	1.00	25.73	C
ATOM	3353	CB	ALA	B	475	23.886	33.075	38.200	1.00	27.00	C
ATOM	3354	C	ALA	B	475	24.680	31.057	39.486	1.00	25.53	C
ATOM	3355	O	ALA	B	475	25.809	31.113	39.970	1.00	26.97	O
ATOM	3356	N	LYS	B	476	24.190	29.953	38.921	1.00	22.58	N
ATOM	3357	CA	LYS	B	476	24.987	28.739	38.771	1.00	23.46	C
ATOM	3358	CB	LYS	B	476	24.594	27.691	39.834	1.00	24.43	C
ATOM	3359	CG	LYS	B	476	25.144	28.000	41.221	1.00	25.55	C
ATOM	3360	CD	LYS	B	476	24.578	26.972	42.233	1.00	32.01	C

ATOM	3361	CE	LYS	B	476	25.288	27.036	43.577	1.00	36.59	C
ATOM	3362	NZ	LYS	B	476	26.553	26.248	43.526	1.00	37.14	N
ATOM	3363	C	LYS	B	476	24.787	28.124	37.402	1.00	24.32	C
ATOM	3364	O	LYS	B	476	23.658	28.084	36.876	1.00	24.88	O
ATOM	3365	N	ILE	B	477	25.869	27.620	36.815	1.00	21.48	N
ATOM	3366	CA	ILE	B	477	25.778	26.980	35.511	1.00	23.09	C
ATOM	3367	CB	ILE	B	477	27.139	26.937	34.843	1.00	20.87	C
ATOM	3368	CG2	ILE	B	477	27.065	26.129	33.544	1.00	24.48	C
ATOM	3369	CG1	ILE	B	477	27.644	28.370	34.642	1.00	22.01	C
ATOM	3370	CD1	ILE	B	477	29.143	28.461	34.443	1.00	23.58	C
ATOM	3371	C	ILE	B	477	25.297	25.560	35.689	1.00	26.88	C
ATOM	3372	O	ILE	B	477	25.794	24.860	36.565	1.00	24.82	O
ATOM	3373	N	SER	B	478	24.351	25.111	34.855	1.00	22.63	N
ATOM	3374	CA	SER	B	478	23.876	23.743	34.992	1.00	23.59	C
ATOM	3375	CB	SER	B	478	22.474	23.741	35.578	1.00	30.50	C
ATOM	3376	OG	SER	B	478	21.607	24.274	34.601	1.00	40.13	O
ATOM	3377	C	SER	B	478	23.842	22.996	33.664	1.00	27.84	C
ATOM	3378	O	SER	B	478	24.253	23.528	32.616	1.00	27.42	O
ATOM	3379	N	ASP	B	479	23.302	21.775	33.730	1.00	23.72	N
ATOM	3380	CA	ASP	B	479	23.164	20.821	32.611	1.00	25.82	C
ATOM	3381	CB	ASP	B	479	22.094	21.256	31.585	1.00	24.35	C
ATOM	3382	CG	ASP	B	479	21.711	20.104	30.636	1.00	34.90	C
ATOM	3383	OD1	ASP	B	479	22.419	19.076	30.636	1.00	30.23	O
ATOM	3384	OD2	ASP	B	479	20.703	20.214	29.899	1.00	30.91	O
ATOM	3385	C	ASP	B	479	24.460	20.489	31.878	1.00	24.50	C
ATOM	3386	O	ASP	B	479	24.751	21.037	30.784	1.00	21.34	O
ATOM	3387	N	PHE	B	480	25.197	19.529	32.444	1.00	26.62	N
ATOM	3388	CA	PHE	B	480	26.464	19.062	31.863	1.00	27.44	C
ATOM	3389	CB	PHE	B	480	27.474	18.812	32.993	1.00	26.01	C
ATOM	3390	CG	PHE	B	480	27.893	20.075	33.696	1.00	25.53	C
ATOM	3391	CD1	PHE	B	480	29.029	20.788	33.289	1.00	37.11	C
ATOM	3392	CD2	PHE	B	480	27.095	20.617	34.700	1.00	30.32	C
ATOM	3393	CE1	PHE	B	480	29.346	22.023	33.870	1.00	34.94	C
ATOM	3394	CE2	PHE	B	480	27.403	21.850	35.279	1.00	31.64	C
ATOM	3395	CZ	PHE	B	480	28.520	22.555	34.866	1.00	33.32	C
ATOM	3396	C	PHE	B	480	26.288	17.810	30.989	1.00	23.32	C
ATOM	3397	O	PHE	B	480	27.242	17.078	30.712	1.00	29.60	O
ATOM	3398	N	GLY	B	481	25.059	17.586	30.533	1.00	24.87	N
ATOM	3399	CA	GLY	B	481	24.743	16.444	29.690	1.00	25.16	C
ATOM	3400	C	GLY	B	481	25.510	16.367	28.377	1.00	32.36	C
ATOM	3401	O	GLY	B	481	25.643	15.300	27.819	1.00	28.44	O
ATOM	3402	N	LEU	B	482	26.017	17.491	27.876	1.00	24.22	N
ATOM	3403	CA	LEU	B	482	26.778	17.474	26.617	1.00	24.32	C
ATOM	3404	CB	LEU	B	482	26.169	18.473	25.622	1.00	27.61	C
ATOM	3405	CG	LEU	B	482	24.767	18.111	25.133	1.00	31.09	C
ATOM	3406	CD1	LEU	B	482	24.143	19.316	24.392	1.00	37.33	C
ATOM	3407	CD2	LEU	B	482	24.868	16.912	24.231	1.00	33.44	C
ATOM	3408	C	LEU	B	482	28.229	17.843	26.833	1.00	20.28	C
ATOM	3409	O	LEU	B	482	28.998	18.006	25.881	1.00	27.53	O
ATOM	3410	N	SER	B	483	28.607	17.986	28.093	1.00	21.03	N
ATOM	3411	CA	SER	B	483	29.959	18.392	28.423	1.00	17.07	C
ATOM	3412	CB	SER	B	483	30.001	18.818	29.882	1.00	21.12	C
ATOM	3413	OG	SER	B	483	29.143	19.933	30.053	1.00	31.09	O
ATOM	3414	C	SER	B	483	30.984	17.298	28.156	1.00	21.12	C
ATOM	3415	O	SER	B	483	30.662	16.131	28.176	1.00	23.30	O
ATOM	3416	N	LYS	B	484	32.225	17.700	27.901	1.00	22.23	N
ATOM	3417	CA	LYS	B	484	33.281	16.732	27.641	1.00	22.46	C
ATOM	3418	CB	LYS	B	484	33.403	16.456	26.135	1.00	25.43	C
ATOM	3419	CG	LYS	B	484	32.202	15.661	25.564	1.00	37.37	C
ATOM	3420	CD	LYS	B	484	32.323	15.382	24.069	1.00	42.87	C
ATOM	3421	CE	LYS	B	484	31.228	14.402	23.622	1.00	42.01	C
ATOM	3422	NZ	LYS	B	484	29.878	14.732	24.149	1.00	57.01	N
ATOM	3423	C	LYS	B	484	34.622	17.227	28.157	1.00	26.66	C
ATOM	3424	O	LYS	B	484	34.870	18.426	28.229	1.00	25.66	O
ATOM	3425	N	ALA	B	485	35.489	16.280	28.492	1.00	22.91	N
ATOM	3426	CA	ALA	B	485	36.825	16.636	28.962	1.00	21.91	C
ATOM	3427	CB	ALA	B	485	37.359	15.560	29.932	1.00	32.95	C
ATOM	3428	C	ALA	B	485	37.689	16.684	27.679	1.00	29.52	C

ATOM	3429	O	ALA	B	485	37.552	15.827	26.804	1.00	32.44	O
ATOM	3430	N	LEU	B	486	38.546	17.694	27.576	1.00	24.43	N
ATOM	3431	CA	LEU	B	486	39.419	17.841	26.403	1.00	19.74	C
ATOM	3432	CB	LEU	B	486	39.663	19.335	26.108	1.00	28.91	C
ATOM	3433	CG	LEU	B	486	38.582	20.155	25.390	1.00	28.77	C
ATOM	3434	CD1	LEU	B	486	38.967	21.633	25.336	1.00	34.39	C
ATOM	3435	CD2	LEU	B	486	38.408	19.629	24.006	1.00	36.84	C
ATOM	3436	C	LEU	B	486	40.794	17.187	26.636	1.00	31.66	C
ATOM	3437	O	LEU	B	486	41.477	16.831	25.690	1.00	34.07	O
ATOM	3438	N	GLY	B	487	41.203	17.066	27.897	1.00	30.25	N
ATOM	3439	CA	GLY	B	487	42.510	16.493	28.177	1.00	35.90	C
ATOM	3440	C	GLY	B	487	43.591	17.425	27.643	1.00	35.05	C
ATOM	3441	O	GLY	B	487	43.547	18.624	27.847	1.00	37.70	O
ATOM	3442	N	ALA	B	488	44.540	16.853	26.919	1.00	36.40	N
ATOM	3443	CA	ALA	B	488	45.644	17.630	26.364	1.00	41.44	C
ATOM	3444	CB	ALA	B	488	46.841	16.711	26.100	1.00	44.00	C
ATOM	3445	C	ALA	B	488	45.283	18.375	25.080	1.00	40.64	C
ATOM	3446	O	ALA	B	488	46.035	19.227	24.627	1.00	40.65	O
ATOM	3447	N	ASP	B	489	44.125	18.068	24.506	1.00	37.22	N
ATOM	3448	CA	ASP	B	489	43.706	18.723	23.255	1.00	35.43	C
ATOM	3449	CB	ASP	B	489	42.740	17.811	22.497	1.00	36.96	C
ATOM	3450	CG	ASP	B	489	43.331	16.450	22.240	1.00	48.65	C
ATOM	3451	OD1	ASP	B	489	44.563	16.383	22.017	1.00	51.66	O
ATOM	3452	OD2	ASP	B	489	42.571	15.457	22.249	1.00	47.30	O
ATOM	3453	C	ASP	B	489	43.062	20.090	23.440	1.00	31.19	C
ATOM	3454	O	ASP	B	489	42.545	20.391	24.502	1.00	31.54	O
ATOM	3455	N	ASP	B	490	43.085	20.911	22.387	1.00	28.93	N
ATOM	3456	CA	ASP	B	490	42.480	22.235	22.480	1.00	31.46	C
ATOM	3457	CB	ASP	B	490	43.333	23.272	21.742	1.00	36.63	C
ATOM	3458	CG	ASP	B	490	43.495	22.950	20.292	1.00	47.74	C
ATOM	3459	OD1	ASP	B	490	44.554	23.298	19.706	1.00	55.99	O
ATOM	3460	OD2	ASP	B	490	42.557	22.364	19.727	1.00	54.77	O
ATOM	3461	C	ASP	B	490	41.047	22.241	21.942	1.00	26.58	C
ATOM	3462	O	ASP	B	490	40.347	23.252	22.028	1.00	25.36	O
ATOM	3463	N	SER	B	491	40.599	21.115	21.398	1.00	24.18	N
ATOM	3464	CA	SER	B	491	39.215	21.008	20.901	1.00	21.95	C
ATOM	3465	CB	SER	B	491	39.067	21.782	19.592	1.00	33.37	C
ATOM	3466	OG	SER	B	491	39.830	21.147	18.559	1.00	33.09	O
ATOM	3467	C	SER	B	491	38.879	19.574	20.619	1.00	29.49	C
ATOM	3468	O	SER	B	491	39.754	18.698	20.726	1.00	26.31	O
ATOM	3469	N	TYR	B	492	37.611	19.310	20.296	1.00	23.30	N
ATOM	3470	CA	TYR	B	492	37.228	17.987	19.891	1.00	24.79	C
ATOM	3471	CB	TYR	B	492	36.708	17.112	21.060	1.00	24.52	C
ATOM	3472	CG	TYR	B	492	35.358	17.507	21.590	1.00	26.67	C
ATOM	3473	CD1	TYR	B	492	34.187	16.946	21.070	1.00	26.01	C
ATOM	3474	CE1	TYR	B	492	32.928	17.362	21.510	1.00	29.14	C
ATOM	3475	CD2	TYR	B	492	35.249	18.487	22.568	1.00	24.91	C
ATOM	3476	CE2	TYR	B	492	33.979	18.912	23.025	1.00	24.00	C
ATOM	3477	CZ	TYR	B	492	32.835	18.343	22.483	1.00	26.42	C
ATOM	3478	OH	TYR	B	492	31.589	18.775	22.887	1.00	26.61	O
ATOM	3479	C	TYR	B	492	36.180	18.166	18.803	1.00	20.40	C
ATOM	3480	O	TYR	B	492	35.632	19.255	18.622	1.00	22.94	O
ATOM	3481	N	TYR	B	493	35.960	17.099	18.050	1.00	20.88	N
ATOM	3482	CA	TYR	B	493	34.958	17.072	16.980	1.00	19.63	C
ATOM	3483	CB	TYR	B	493	35.559	16.596	15.671	1.00	21.26	C
ATOM	3484	CG	TYR	B	493	36.515	17.601	15.095	1.00	24.50	C
ATOM	3485	CD1	TYR	B	493	37.777	17.769	15.645	1.00	27.04	C
ATOM	3486	CE1	TYR	B	493	38.652	18.713	15.144	1.00	36.13	C
ATOM	3487	CD2	TYR	B	493	36.137	18.407	14.014	1.00	26.33	C
ATOM	3488	CE2	TYR	B	493	37.011	19.352	13.501	1.00	27.99	C
ATOM	3489	CZ	TYR	B	493	38.262	19.497	14.067	1.00	32.35	C
ATOM	3490	OH	TYR	B	493	39.144	20.396	13.526	1.00	33.44	O
ATOM	3491	C	TYR	B	493	33.944	16.069	17.468	1.00	21.80	C
ATOM	3492	O	TYR	B	493	34.293	14.925	17.800	1.00	22.36	O
ATOM	3493	N	THR	B	494	32.695	16.514	17.539	1.00	26.46	N
ATOM	3494	CA	THR	B	494	31.623	15.700	18.095	1.00	33.93	C
ATOM	3495	CB	THR	B	494	30.580	16.611	18.817	1.00	33.02	C
ATOM	3496	OG1	THR	B	494	29.647	15.794	19.538	1.00	40.25	O

ATOM	3497	CG2	THR	B	494	29.817	17.435	17.812	1.00	33.65	C
ATOM	3498	C	THR	B	494	30.875	14.851	17.104	1.00	36.70	C
ATOM	3499	O	THR	B	494	30.757	15.179	15.921	1.00	28.58	O
ATOM	3500	N	ALA	B	495	30.294	13.773	17.611	1.00	44.45	N
ATOM	3501	CA	ALA	B	495	29.508	12.911	16.764	1.00	49.14	C
ATOM	3502	CB	ALA	B	495	29.442	11.529	17.370	1.00	47.66	C
ATOM	3503	C	ALA	B	495	28.108	13.503	16.624	1.00	49.65	C
ATOM	3504	O	ALA	B	495	27.651	14.233	17.498	1.00	48.99	O
ATOM	3505	N	ARG	B	496	27.446	13.194	15.519	1.00	53.97	N
ATOM	3506	CA	ARG	B	496	26.098	13.678	15.264	1.00	57.66	C
ATOM	3507	CB	ARG	B	496	25.804	13.674	13.759	1.00	60.80	C
ATOM	3508	CG	ARG	B	496	25.116	14.929	13.230	1.00	65.91	C
ATOM	3509	CD	ARG	B	496	23.905	15.299	14.043	1.00	66.81	C
ATOM	3510	NE	ARG	B	496	23.322	16.552	13.573	1.00	66.60	N
ATOM	3511	CZ	ARG	B	496	22.295	17.160	14.156	1.00	71.04	C
ATOM	3512	NH1	ARG	B	496	21.737	16.626	15.237	1.00	70.95	N
ATOM	3513	NH2	ARG	B	496	21.826	18.299	13.660	1.00	66.70	N
ATOM	3514	C	ARG	B	496	25.106	12.741	15.964	1.00	60.28	C
ATOM	3515	O	ARG	B	496	25.185	11.519	15.826	1.00	58.20	O
ATOM	3516	N	SER	B	497	24.183	13.316	16.721	1.00	58.58	N
ATOM	3517	CA	SER	B	497	23.175	12.513	17.407	1.00	60.66	C
ATOM	3518	CB	SER	B	497	23.267	12.711	18.920	1.00	58.31	C
ATOM	3519	OG	SER	B	497	22.882	14.026	19.276	1.00	66.25	O
ATOM	3520	C	SER	B	497	21.809	12.965	16.913	1.00	60.66	C
ATOM	3521	O	SER	B	497	21.711	13.896	16.114	1.00	59.92	O
ATOM	3522	N	ALA	B	498	20.764	12.305	17.396	1.00	63.28	N
ATOM	3523	CA	ALA	B	498	19.399	12.645	17.015	1.00	61.54	C
ATOM	3524	CB	ALA	B	498	18.440	11.531	17.450	1.00	58.15	C
ATOM	3525	C	ALA	B	498	18.995	13.963	17.671	1.00	60.15	C
ATOM	3526	O	ALA	B	498	19.422	14.275	18.783	1.00	59.70	O
ATOM	3527	N	GLY	B	499	18.168	14.733	16.977	1.00	61.09	N
ATOM	3528	CA	GLY	B	499	17.719	15.994	17.533	1.00	63.27	C
ATOM	3529	C	GLY	B	499	18.325	17.184	16.826	1.00	61.70	C
ATOM	3530	O	GLY	B	499	19.309	17.051	16.096	1.00	63.96	O
ATOM	3531	N	LYS	B	500	17.735	18.352	17.042	1.00	59.76	N
ATOM	3532	CA	LYS	B	500	18.216	19.576	16.417	1.00	57.53	C
ATOM	3533	CB	LYS	B	500	17.052	20.550	16.210	1.00	60.45	C
ATOM	3534	CG	LYS	B	500	16.017	20.091	15.199	1.00	61.48	C
ATOM	3535	CD	LYS	B	500	16.561	20.185	13.780	1.00	65.74	C
ATOM	3536	CE	LYS	B	500	15.500	19.800	12.756	1.00	62.41	C
ATOM	3537	NZ	LYS	B	500	16.013	19.898	11.358	1.00	67.47	N
ATOM	3538	C	LYS	B	500	19.283	20.251	17.275	1.00	51.49	C
ATOM	3539	O	LYS	B	500	19.282	20.137	18.495	1.00	49.86	O
ATOM	3540	N	TRP	B	501	20.195	20.957	16.618	1.00	45.23	N
ATOM	3541	CA	TRP	B	501	21.253	21.680	17.325	1.00	46.44	C
ATOM	3542	CB	TRP	B	501	22.530	21.673	16.483	1.00	40.73	C
ATOM	3543	CG	TRP	B	501	23.332	20.423	16.584	1.00	38.73	C
ATOM	3544	CD2	TRP	B	501	24.704	20.258	16.199	1.00	35.99	C
ATOM	3545	CE2	TRP	B	501	25.085	18.943	16.562	1.00	39.61	C
ATOM	3546	CE3	TRP	B	501	25.651	21.095	15.586	1.00	39.41	C
ATOM	3547	CD1	TRP	B	501	22.942	19.235	17.133	1.00	40.88	C
ATOM	3548	NE1	TRP	B	501	23.992	18.339	17.130	1.00	40.09	N
ATOM	3549	CZ2	TRP	B	501	26.375	18.448	16.337	1.00	35.77	C
ATOM	3550	CZ3	TRP	B	501	26.942	20.597	15.361	1.00	34.28	C
ATOM	3551	CH2	TRP	B	501	27.286	19.287	15.739	1.00	40.15	C
ATOM	3552	C	TRP	B	501	20.795	23.126	17.545	1.00	39.13	C
ATOM	3553	O	TRP	B	501	20.193	23.722	16.648	1.00	42.06	O
ATOM	3554	N	PRO	B	502	21.060	23.703	18.736	1.00	35.62	N
ATOM	3555	CD	PRO	B	502	21.732	23.060	19.884	1.00	36.26	C
ATOM	3556	CA	PRO	B	502	20.675	25.094	19.056	1.00	38.57	C
ATOM	3557	CB	PRO	B	502	20.841	25.158	20.569	1.00	36.44	C
ATOM	3558	CG	PRO	B	502	22.021	24.232	20.803	1.00	42.17	C
ATOM	3559	C	PRO	B	502	21.650	26.019	18.328	1.00	34.08	C
ATOM	3560	O	PRO	B	502	22.528	26.650	18.941	1.00	27.50	O
ATOM	3561	N	LEU	B	503	21.487	26.069	17.011	1.00	27.87	N
ATOM	3562	CA	LEU	B	503	22.377	26.847	16.147	1.00	30.99	C
ATOM	3563	CB	LEU	B	503	21.846	26.834	14.706	1.00	35.93	C
ATOM	3564	CG	LEU	B	503	21.555	25.457	14.117	1.00	38.86	C

ATOM	3565	CD1	LEU	B	503	20.943	25.607	12.720	1.00	46.43	C
ATOM	3566	CD2	LEU	B	503	22.833	24.656	14.046	1.00	42.19	C
ATOM	3567	C	LEU	B	503	22.603	28.287	16.564	1.00	24.64	C
ATOM	3568	O	LEU	B	503	23.707	28.826	16.364	1.00	24.20	O
ATOM	3569	N	LYS	B	504	21.586	28.914	17.154	1.00	24.76	N
ATOM	3570	CA	LYS	B	504	21.712	30.313	17.542	1.00	26.03	C
ATOM	3571	CB	LYS	B	504	20.353	30.890	17.939	1.00	29.28	C
ATOM	3572	CG	LYS	B	504	19.400	31.000	16.729	1.00	31.16	C
ATOM	3573	CD	LYS	B	504	18.070	31.656	17.108	1.00	33.06	C
ATOM	3574	CE	LYS	B	504	17.121	31.755	15.913	1.00	34.32	C
ATOM	3575	NZ	LYS	B	504	15.941	32.606	16.264	1.00	37.82	N
ATOM	3576	C	LYS	B	504	22.726	30.552	18.657	1.00	28.80	C
ATOM	3577	O	LYS	B	504	23.130	31.663	18.884	1.00	20.01	O
ATOM	3578	N	TRP	B	505	23.141	29.497	19.338	1.00	23.22	N
ATOM	3579	CA	TRP	B	505	24.134	29.656	20.408	1.00	19.35	C
ATOM	3580	CB	TRP	B	505	23.681	28.883	21.665	1.00	25.81	C
ATOM	3581	CG	TRP	B	505	22.680	29.620	22.472	1.00	24.36	C
ATOM	3582	CD2	TRP	B	505	21.277	29.724	22.215	1.00	22.43	C
ATOM	3583	CE2	TRP	B	505	20.739	30.586	23.194	1.00	23.82	C
ATOM	3584	CE3	TRP	B	505	20.415	29.170	21.251	1.00	27.42	C
ATOM	3585	CD1	TRP	B	505	22.934	30.389	23.567	1.00	18.37	C
ATOM	3586	NE1	TRP	B	505	21.771	30.980	24.005	1.00	23.48	N
ATOM	3587	CZ2	TRP	B	505	19.371	30.916	23.245	1.00	31.39	C
ATOM	3588	CZ3	TRP	B	505	19.051	29.496	21.299	1.00	28.93	C
ATOM	3589	CH2	TRP	B	505	18.547	30.365	22.296	1.00	25.25	C
ATOM	3590	C	TRP	B	505	25.497	29.098	19.954	1.00	19.69	C
ATOM	3591	O	TRP	B	505	26.496	29.233	20.663	1.00	22.22	O
ATOM	3592	N	TYR	B	506	25.546	28.513	18.767	1.00	21.76	N
ATOM	3593	CA	TYR	B	506	26.794	27.885	18.285	1.00	22.94	C
ATOM	3594	CB	TYR	B	506	26.426	26.615	17.488	1.00	21.82	C
ATOM	3595	CG	TYR	B	506	26.093	25.389	18.339	1.00	23.08	C
ATOM	3596	CD1	TYR	B	506	25.885	25.496	19.710	1.00	25.11	C
ATOM	3597	CE1	TYR	B	506	25.559	24.358	20.489	1.00	34.90	C
ATOM	3598	CD2	TYR	B	506	25.981	24.124	17.751	1.00	29.64	C
ATOM	3599	CE2	TYR	B	506	25.669	22.993	18.524	1.00	32.44	C
ATOM	3600	CZ	TYR	B	506	25.454	23.117	19.880	1.00	32.19	C
ATOM	3601	OH	TYR	B	506	25.086	22.008	20.619	1.00	37.37	O
ATOM	3602	C	TYR	B	506	27.745	28.757	17.434	1.00	28.60	C
ATOM	3603	O	TYR	B	506	27.299	29.447	16.524	1.00	25.58	O
ATOM	3604	N	ALA	B	507	29.048	28.703	17.731	1.00	23.48	N
ATOM	3605	CA	ALA	B	507	30.061	29.440	16.980	1.00	22.63	C
ATOM	3606	CB	ALA	B	507	31.443	29.298	17.674	1.00	19.24	C
ATOM	3607	C	ALA	B	507	30.122	28.845	15.567	1.00	24.54	C
ATOM	3608	O	ALA	B	507	29.709	27.709	15.343	1.00	23.92	O
ATOM	3609	N	PRO	B	508	30.659	29.597	14.603	1.00	22.52	N
ATOM	3610	CD	PRO	B	508	31.136	30.985	14.747	1.00	24.20	C
ATOM	3611	CA	PRO	B	508	30.772	29.135	13.212	1.00	23.99	C
ATOM	3612	CB	PRO	B	508	31.546	30.265	12.529	1.00	28.71	C
ATOM	3613	CG	PRO	B	508	31.113	31.477	13.328	1.00	35.43	C
ATOM	3614	C	PRO	B	508	31.452	27.787	13.007	1.00	23.80	C
ATOM	3615	O	PRO	B	508	30.960	26.964	12.231	1.00	23.69	O
ATOM	3616	N	GLU	B	509	32.576	27.568	13.695	1.00	22.83	N
ATOM	3617	CA	GLU	B	509	33.316	26.315	13.564	1.00	26.16	C
ATOM	3618	CB	GLU	B	509	34.689	26.390	14.268	1.00	26.11	C
ATOM	3619	CG	GLU	B	509	34.622	26.429	15.792	1.00	25.28	C
ATOM	3620	CD	GLU	B	509	34.538	27.843	16.341	1.00	30.45	C
ATOM	3621	OE1	GLU	B	509	34.270	28.798	15.561	1.00	24.15	O
ATOM	3622	OE2	GLU	B	509	34.716	27.989	17.568	1.00	25.31	O
ATOM	3623	C	GLU	B	509	32.512	25.128	14.098	1.00	22.82	C
ATOM	3624	O	GLU	B	509	32.751	23.992	13.686	1.00	25.61	O
ATOM	3625	N	CYS	B	510	31.571	25.389	15.010	1.00	20.67	N
ATOM	3626	CA	CYS	B	510	30.726	24.323	15.536	1.00	17.87	C
ATOM	3627	CB	CYS	B	510	29.867	24.838	16.704	1.00	17.65	C
ATOM	3628	SG	CYS	B	510	30.852	25.448	18.085	1.00	24.98	S
ATOM	3629	C	CYS	B	510	29.772	23.849	14.428	1.00	20.96	C
ATOM	3630	O	CYS	B	510	29.602	22.676	14.188	1.00	25.35	O
ATOM	3631	N	ILE	B	511	29.149	24.803	13.763	1.00	21.34	N
ATOM	3632	CA	ILE	B	511	28.188	24.473	12.713	1.00	26.63	C

ATOM	3633	CB	ILE	B	511	27.286	25.707	12.388	1.00	27.47	C
ATOM	3634	CG2	ILE	B	511	26.264	25.345	11.289	1.00	33.99	C
ATOM	3635	CG1	ILE	B	511	26.574	26.153	13.671	1.00	26.92	C
ATOM	3636	CD1	ILE	B	511	25.895	27.516	13.597	1.00	31.85	C
ATOM	3637	C	ILE	B	511	28.871	23.984	11.446	1.00	30.34	C
ATOM	3638	O	ILE	B	511	28.434	22.987	10.848	1.00	29.71	O
ATOM	3639	N	ASN	B	512	29.968	24.623	11.058	1.00	25.07	N
ATOM	3640	CA	ASN	B	512	30.615	24.223	9.825	1.00	25.52	C
ATOM	3641	CB	ASN	B	512	31.416	25.376	9.236	1.00	23.08	C
ATOM	3642	CG	ASN	B	512	30.539	26.534	8.817	1.00	31.89	C
ATOM	3643	OD1	ASN	B	512	29.466	26.336	8.268	1.00	35.21	O
ATOM	3644	ND2	ASN	B	512	31.000	27.747	9.072	1.00	40.49	N
ATOM	3645	C	ASN	B	512	31.518	23.014	9.970	1.00	30.37	C
ATOM	3646	O	ASN	B	512	31.633	22.224	9.045	1.00	30.30	O
ATOM	3647	N	PHE	B	513	32.178	22.874	11.109	1.00	23.05	N
ATOM	3648	CA	PHE	B	513	33.084	21.744	11.273	1.00	21.06	C
ATOM	3649	CB	PHE	B	513	34.513	22.245	11.303	1.00	21.42	C
ATOM	3650	CG	PHE	B	513	34.924	22.945	10.031	1.00	32.74	C
ATOM	3651	CD1	PHE	B	513	35.063	24.326	10.005	1.00	34.47	C
ATOM	3652	CD2	PHE	B	513	35.120	22.216	8.858	1.00	32.93	C
ATOM	3653	CE1	PHE	B	513	35.393	24.986	8.805	1.00	39.39	C
ATOM	3654	CE2	PHE	B	513	35.448	22.871	7.664	1.00	40.01	C
ATOM	3655	CZ	PHE	B	513	35.581	24.253	7.645	1.00	36.34	C
ATOM	3656	C	PHE	B	513	32.856	20.836	12.477	1.00	24.61	C
ATOM	3657	O	PHE	B	513	33.687	19.968	12.741	1.00	25.10	O
ATOM	3658	N	ARG	B	514	31.758	21.060	13.207	1.00	20.51	N
ATOM	3659	CA	ARG	B	514	31.407	20.266	14.381	1.00	21.86	C
ATOM	3660	CB	ARG	B	514	31.062	18.815	13.944	1.00	21.50	C
ATOM	3661	CG	ARG	B	514	29.938	18.782	12.935	1.00	22.64	C
ATOM	3662	CD	ARG	B	514	29.437	17.415	12.570	1.00	25.89	C
ATOM	3663	NE	ARG	B	514	28.284	17.550	11.668	1.00	25.50	N
ATOM	3664	CZ	ARG	B	514	27.531	16.537	11.265	1.00	27.87	C
ATOM	3665	NH1	ARG	B	514	27.803	15.306	11.672	1.00	28.30	N
ATOM	3666	NH2	ARG	B	514	26.476	16.760	10.478	1.00	28.78	N
ATOM	3667	C	ARG	B	514	32.560	20.260	15.395	1.00	21.80	C
ATOM	3668	O	ARG	B	514	32.735	19.299	16.141	1.00	23.13	O
ATOM	3669	N	LYS	B	515	33.288	21.373	15.438	1.00	23.39	N
ATOM	3670	CA	LYS	B	515	34.442	21.512	16.323	1.00	21.15	C
ATOM	3671	CB	LYS	B	515	35.551	22.203	15.532	1.00	22.48	C
ATOM	3672	CG	LYS	B	515	36.848	22.399	16.309	1.00	23.37	C
ATOM	3673	CD	LYS	B	515	37.848	23.195	15.490	1.00	30.48	C
ATOM	3674	CE	LYS	B	515	38.992	23.662	16.372	1.00	37.06	C
ATOM	3675	NZ	LYS	B	515	39.892	24.621	15.659	1.00	43.43	N
ATOM	3676	C	LYS	B	515	34.100	22.315	17.597	1.00	22.11	C
ATOM	3677	O	LYS	B	515	33.704	23.477	17.503	1.00	20.32	O
ATOM	3678	N	PHE	B	516	34.302	21.712	18.773	1.00	22.31	N
ATOM	3679	CA	PHE	B	516	33.987	22.381	20.045	1.00	19.14	C
ATOM	3680	CB	PHE	B	516	32.903	21.592	20.788	1.00	20.60	C
ATOM	3681	CG	PHE	B	516	31.585	21.555	20.037	1.00	21.15	C
ATOM	3682	CD1	PHE	B	516	31.411	20.683	18.963	1.00	22.16	C
ATOM	3683	CD2	PHE	B	516	30.559	22.439	20.371	1.00	25.22	C
ATOM	3684	CE1	PHE	B	516	30.223	20.683	18.229	1.00	25.00	C
ATOM	3685	CE2	PHE	B	516	29.374	22.450	19.629	1.00	23.08	C
ATOM	3686	CZ	PHE	B	516	29.209	21.565	18.561	1.00	27.70	C
ATOM	3687	C	PHE	B	516	35.214	22.578	20.911	1.00	19.07	C
ATOM	3688	O	PHE	B	516	36.127	21.736	20.908	1.00	21.35	O
ATOM	3689	N	SER	B	517	35.206	23.667	21.684	1.00	19.27	N
ATOM	3690	CA	SER	B	517	36.366	24.059	22.496	1.00	26.23	C
ATOM	3691	CB	SER	B	517	37.385	24.718	21.542	1.00	24.44	C
ATOM	3692	OG	SER	B	517	36.770	25.861	20.910	1.00	22.44	O
ATOM	3693	C	SER	B	517	35.935	25.102	23.528	1.00	21.53	C
ATOM	3694	O	SER	B	517	34.792	25.509	23.523	1.00	20.37	O
ATOM	3695	N	SER	B	518	36.836	25.554	24.404	1.00	19.72	N
ATOM	3696	CA	SER	B	518	36.435	26.590	25.329	1.00	20.34	C
ATOM	3697	CB	SER	B	518	37.555	26.890	26.341	1.00	27.31	C
ATOM	3698	OG	SER	B	518	37.592	25.809	27.275	1.00	32.37	O
ATOM	3699	C	SER	B	518	36.039	27.842	24.551	1.00	21.23	C
ATOM	3700	O	SER	B	518	35.165	28.589	24.977	1.00	23.54	O

ATOM	3701	N	ARG	B	519	36.689	28.055	23.421	1.00	21.32	N
ATOM	3702	CA	ARG	B	519	36.347	29.205	22.610	1.00	18.97	C
ATOM	3703	CB	ARG	B	519	37.414	29.420	21.545	1.00	21.22	C
ATOM	3704	CG	ARG	B	519	38.585	30.196	22.148	1.00	26.38	C
ATOM	3705	CD	ARG	B	519	39.753	30.191	21.208	1.00	35.68	C
ATOM	3706	NE	ARG	B	519	40.851	30.943	21.789	1.00	42.06	N
ATOM	3707	CZ	ARG	B	519	42.082	30.952	21.288	1.00	46.57	C
ATOM	3708	NH1	ARG	B	519	42.367	30.246	20.195	1.00	43.72	N
ATOM	3709	NH2	ARG	B	519	43.032	31.653	21.892	1.00	49.64	N
ATOM	3710	C	ARG	B	519	34.964	29.121	21.987	1.00	19.81	C
ATOM	3711	O	ARG	B	519	34.363	30.171	21.729	1.00	21.27	O
ATOM	3712	N	SER	B	520	34.460	27.909	21.718	1.00	18.58	N
ATOM	3713	CA	SER	B	520	33.075	27.864	21.213	1.00	21.84	C
ATOM	3714	CB	SER	B	520	32.742	26.535	20.503	1.00	20.81	C
ATOM	3715	OG	SER	B	520	32.908	25.379	21.297	1.00	22.92	O
ATOM	3716	C	SER	B	520	32.158	28.162	22.437	1.00	23.07	C
ATOM	3717	O	SER	B	520	31.091	28.760	22.290	1.00	21.17	O
ATOM	3718	N	ASP	B	521	32.597	27.810	23.649	1.00	19.80	N
ATOM	3719	CA	ASP	B	521	31.824	28.119	24.877	1.00	21.41	C
ATOM	3720	CB	ASP	B	521	32.462	27.523	26.150	1.00	28.78	C
ATOM	3721	CG	ASP	B	521	32.050	26.058	26.409	1.00	22.85	C
ATOM	3722	OD1	ASP	B	521	31.099	25.558	25.763	1.00	22.20	O
ATOM	3723	OD2	ASP	B	521	32.683	25.426	27.306	1.00	22.04	O
ATOM	3724	C	ASP	B	521	31.827	29.656	25.044	1.00	17.40	C
ATOM	3725	O	ASP	B	521	30.822	30.257	25.477	1.00	20.22	O
ATOM	3726	N	VAL	B	522	32.944	30.299	24.673	1.00	16.61	N
ATOM	3727	CA	VAL	B	522	32.990	31.785	24.758	1.00	15.75	C
ATOM	3728	CB	VAL	B	522	34.397	32.326	24.385	1.00	18.63	C
ATOM	3729	CG1	VAL	B	522	34.392	33.849	24.190	1.00	20.55	C
ATOM	3730	CG2	VAL	B	522	35.377	31.957	25.537	1.00	18.25	C
ATOM	3731	C	VAL	B	522	31.927	32.402	23.834	1.00	16.27	C
ATOM	3732	O	VAL	B	522	31.243	33.352	24.221	1.00	18.90	O
ATOM	3733	N	TRP	B	523	31.783	31.848	22.634	1.00	17.66	N
ATOM	3734	CA	TRP	B	523	30.758	32.371	21.708	1.00	16.82	C
ATOM	3735	CB	TRP	B	523	30.805	31.584	20.386	1.00	15.58	C
ATOM	3736	CG	TRP	B	523	29.813	32.106	19.335	1.00	17.41	C
ATOM	3737	CD2	TRP	B	523	30.129	32.847	18.145	1.00	19.38	C
ATOM	3738	CE2	TRP	B	523	28.904	33.164	17.516	1.00	20.03	C
ATOM	3739	CE3	TRP	B	523	31.332	33.280	17.546	1.00	18.44	C
ATOM	3740	CD1	TRP	B	523	28.448	31.999	19.375	1.00	22.97	C
ATOM	3741	NE1	TRP	B	523	27.891	32.641	18.280	1.00	18.65	N
ATOM	3742	CZ2	TRP	B	523	28.839	33.895	16.322	1.00	21.60	C
ATOM	3743	CZ3	TRP	B	523	31.263	34.010	16.359	1.00	19.75	C
ATOM	3744	CH2	TRP	B	523	30.030	34.313	15.758	1.00	19.91	C
ATOM	3745	C	TRP	B	523	29.373	32.241	22.358	1.00	18.12	C
ATOM	3746	O	TRP	B	523	28.573	33.189	22.321	1.00	19.38	O
ATOM	3747	N	SER	B	524	29.088	31.082	22.956	1.00	17.71	N
ATOM	3748	CA	SER	B	524	27.791	30.853	23.643	1.00	22.69	C
ATOM	3749	CB	SER	B	524	27.740	29.419	24.213	1.00	21.28	C
ATOM	3750	OG	SER	B	524	27.817	28.467	23.185	1.00	31.98	O
ATOM	3751	C	SER	B	524	27.579	31.829	24.792	1.00	22.41	C
ATOM	3752	O	SER	B	524	26.464	32.331	25.014	1.00	18.61	O
ATOM	3753	N	TYR	B	525	28.644	32.099	25.546	1.00	22.85	N
ATOM	3754	CA	TYR	B	525	28.619	33.051	26.640	1.00	21.01	C
ATOM	3755	CB	TYR	B	525	30.040	33.201	27.268	1.00	19.16	C
ATOM	3756	CG	TYR	B	525	30.046	34.181	28.409	1.00	20.09	C
ATOM	3757	CD1	TYR	B	525	29.456	33.865	29.638	1.00	21.83	C
ATOM	3758	CE1	TYR	B	525	29.411	34.806	30.692	1.00	20.51	C
ATOM	3759	CD2	TYR	B	525	30.602	35.461	28.251	1.00	19.44	C
ATOM	3760	CE2	TYR	B	525	30.553	36.400	29.286	1.00	21.12	C
ATOM	3761	CZ	TYR	B	525	29.956	36.066	30.501	1.00	26.32	C
ATOM	3762	OH	TYR	B	525	29.911	36.999	31.518	1.00	24.81	O
ATOM	3763	C	TYR	B	525	28.159	34.407	26.098	1.00	20.91	C
ATOM	3764	O	TYR	B	525	27.344	35.092	26.718	1.00	20.39	O
ATOM	3765	N	GLY	B	526	28.711	34.811	24.950	1.00	18.42	N
ATOM	3766	CA	GLY	B	526	28.306	36.086	24.357	1.00	19.09	C
ATOM	3767	C	GLY	B	526	26.803	36.116	24.081	1.00	16.71	C
ATOM	3768	O	GLY	B	526	26.135	37.118	24.371	1.00	19.95	O

ATOM	3769	N	VAL	B	527	26.271	35.039	23.506	1.00 19.63	N
ATOM	3770	CA	VAL	B	527	24.821	34.980	23.240	1.00 17.92	C
ATOM	3771	CB	VAL	B	527	24.470	33.705	22.461	1.00 18.12	C
ATOM	3772	CG1	VAL	B	527	22.943	33.645	22.145	1.00 19.94	C
ATOM	3773	CG2	VAL	B	527	25.270	33.697	21.122	1.00 19.40	C
ATOM	3774	C	VAL	B	527	24.082	35.026	24.600	1.00 20.57	C
ATOM	3775	O	VAL	B	527	23.063	35.686	24.735	1.00 21.39	O
ATOM	3776	N	THR	B	528	24.633	34.377	25.619	1.00 20.54	N
ATOM	3777	CA	THR	B	528	24.010	34.397	26.949	1.00 18.80	C
ATOM	3778	CB	THR	B	528	24.768	33.458	27.906	1.00 20.59	C
ATOM	3779	OG1	THR	B	528	24.673	32.114	27.395	1.00 21.50	O
ATOM	3780	CG2	THR	B	528	24.169	33.499	29.287	1.00 22.95	C
ATOM	3781	C	THR	B	528	23.981	35.821	27.507	1.00 25.29	C
ATOM	3782	O	THR	B	528	22.972	36.235	28.084	1.00 19.03	O
ATOM	3783	N	MET	B	529	25.083	36.560	27.337	1.00 21.53	N
ATOM	3784	CA	MET	B	529	25.147	37.955	27.789	1.00 20.49	C
ATOM	3785	CB	MET	B	529	26.479	38.621	27.360	1.00 20.90	C
ATOM	3786	CG	MET	B	529	27.726	38.072	28.092	1.00 22.65	C
ATOM	3787	SD	MET	B	529	29.178	39.101	27.591	1.00 24.81	S
ATOM	3788	CE	MET	B	529	28.792	40.693	28.291	1.00 22.12	C
ATOM	3789	C	MET	B	529	24.013	38.740	27.103	1.00 19.53	C
ATOM	3790	O	MET	B	529	23.331	39.551	27.739	1.00 20.14	O
ATOM	3791	N	TRP	B	530	23.843	38.505	25.802	1.00 20.92	N
ATOM	3792	CA	TRP	B	530	22.800	39.234	25.035	1.00 19.60	C
ATOM	3793	CB	TRP	B	530	22.848	38.845	23.556	1.00 20.03	C
ATOM	3794	CG	TRP	B	530	21.996	39.725	22.693	1.00 18.41	C
ATOM	3795	CD2	TRP	B	530	20.610	39.533	22.395	1.00 19.07	C
ATOM	3796	CE2	TRP	B	530	20.191	40.635	21.590	1.00 20.94	C
ATOM	3797	CE3	TRP	B	530	19.678	38.543	22.726	1.00 22.34	C
ATOM	3798	CD1	TRP	B	530	22.373	40.909	22.072	1.00 18.66	C
ATOM	3799	NE1	TRP	B	530	21.276	41.460	21.399	1.00 21.22	N
ATOM	3800	CZ2	TRP	B	530	18.866	40.762	21.116	1.00 26.05	C
ATOM	3801	CZ3	TRP	B	530	18.369	38.673	22.254	1.00 23.03	C
ATOM	3802	CH2	TRP	B	530	17.978	39.770	21.462	1.00 27.41	C
ATOM	3803	C	TRP	B	530	21.403	38.947	25.567	1.00 21.14	C
ATOM	3804	O	TRP	B	530	20.607	39.880	25.807	1.00 22.19	O
ATOM	3805	N	GLU	B	531	21.101	37.665	25.754	1.00 21.34	N
ATOM	3806	CA	GLU	B	531	19.799	37.234	26.288	1.00 22.58	C
ATOM	3807	CB	GLU	B	531	19.785	35.725	26.566	1.00 23.47	C
ATOM	3808	CG	GLU	B	531	19.941	34.786	25.384	1.00 26.14	C
ATOM	3809	CD	GLU	B	531	19.873	33.318	25.844	1.00 26.77	C
ATOM	3810	OE1	GLU	B	531	20.953	32.715	26.078	1.00 22.88	O
ATOM	3811	OE2	GLU	B	531	18.731	32.788	25.983	1.00 27.11	O
ATOM	3812	C	GLU	B	531	19.548	37.897	27.617	1.00 20.02	C
ATOM	3813	O	GLU	B	531	18.432	38.384	27.895	1.00 23.77	O
ATOM	3814	N	ALA	B	532	20.565	37.903	28.478	1.00 20.17	N
ATOM	3815	CA	ALA	B	532	20.408	38.497	29.795	1.00 18.65	C
ATOM	3816	CB	ALA	B	532	21.617	38.155	30.711	1.00 20.90	C
ATOM	3817	C	ALA	B	532	20.204	39.994	29.776	1.00 24.11	C
ATOM	3818	O	ALA	B	532	19.290	40.506	30.425	1.00 20.67	O
ATOM	3819	N	LEU	B	533	21.062	40.701	29.045	1.00 24.27	N
ATOM	3820	CA	LEU	B	533	20.980	42.163	28.975	1.00 28.04	C
ATOM	3821	CB	LEU	B	533	22.282	42.737	28.376	1.00 22.81	C
ATOM	3822	CG	LEU	B	533	23.472	42.615	29.345	1.00 21.62	C
ATOM	3823	CD1	LEU	B	533	24.801	42.869	28.608	1.00 29.89	C
ATOM	3824	CD2	LEU	B	533	23.309	43.620	30.508	1.00 25.39	C
ATOM	3825	C	LEU	B	533	19.745	42.629	28.194	1.00 26.38	C
ATOM	3826	O	LEU	B	533	19.352	43.810	28.275	1.00 22.57	O
ATOM	3827	N	SER	B	534	19.122	41.702	27.464	1.00 21.44	N
ATOM	3828	CA	SER	B	534	17.888	41.991	26.714	1.00 23.07	C
ATOM	3829	CB	SER	B	534	17.862	41.187	25.429	1.00 21.95	C
ATOM	3830	OG	SER	B	534	18.842	41.679	24.534	1.00 31.02	O
ATOM	3831	C	SER	B	534	16.709	41.560	27.562	1.00 24.51	C
ATOM	3832	O	SER	B	534	15.571	41.538	27.106	1.00 27.12	O
ATOM	3833	N	TYR	B	535	17.000	41.199	28.803	1.00 25.92	N
ATOM	3834	CA	TYR	B	535	15.990	40.738	29.739	1.00 28.32	C
ATOM	3835	CB	TYR	B	535	15.102	41.910	30.198	1.00 28.47	C
ATOM	3836	CG	TYR	B	535	15.858	42.811	31.144	1.00 29.31	C

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ATOM   3837  CD1 TYR B 535      16.777  43.733  30.652  1.00 28.02           C
ATOM   3838  CE1 TYR B 535      17.563  44.492  31.511  1.00 29.55           C
ATOM   3839  CD2 TYR B 535      15.736  42.679  32.526  1.00 28.97           C
ATOM   3840  CE2 TYR B 535      16.514  43.434  33.395  1.00 30.17           C
ATOM   3841  CZ  TYR B 535      17.431  44.341  32.874  1.00 22.54           C
ATOM   3842  OH  TYR B 535      18.185  45.117  33.713  1.00 29.23           O
ATOM   3843  C   TYR B 535      15.137  39.579  29.224  1.00 30.50           C
ATOM   3844  O   TYR B 535      13.918  39.637  29.245  1.00 29.15           O
ATOM   3845  N   GLY B 536      15.805  38.525  28.754  1.00 25.34           N
ATOM   3846  CA  GLY B 536      15.090  37.334  28.313  1.00 26.66           C
ATOM   3847  C   GLY B 536      14.563  37.236  26.907  1.00 28.90           C
ATOM   3848  O   GLY B 536      13.831  36.301  26.583  1.00 34.84           O
ATOM   3849  N   GLN B 537      14.940  38.177  26.044  1.00 30.40           N
ATOM   3850  CA  GLN B 537      14.504  38.138  24.658  1.00 28.41           C
ATOM   3851  CB  GLN B 537      14.840  39.463  23.973  1.00 32.82           C
ATOM   3852  CG  GLN B 537      13.837  40.571  24.309  1.00 43.11           C
ATOM   3853  CD  GLN B 537      14.217  41.920  23.731  1.00 47.65           C
ATOM   3854  OE1 GLN B 537      14.599  42.029  22.562  1.00 54.72           O
ATOM   3855  NE2 GLN B 537      14.108  42.961  24.547  1.00 50.31           N
ATOM   3856  C   GLN B 537      15.175  36.979  23.918  1.00 30.53           C
ATOM   3857  O   GLN B 537      16.238  36.507  24.326  1.00 25.81           O
ATOM   3858  N   LYS B 538      14.550  36.515  22.832  1.00 26.52           N
ATOM   3859  CA  LYS B 538      15.124  35.429  22.060  1.00 26.82           C
ATOM   3860  CB  LYS B 538      14.036  34.673  21.292  1.00 33.23           C
ATOM   3861  CG  LYS B 538      13.077  33.922  22.201  1.00 43.54           C
ATOM   3862  CD  LYS B 538      12.031  33.160  21.393  1.00 44.85           C
ATOM   3863  CE  LYS B 538      11.278  32.173  22.282  1.00 50.77           C
ATOM   3864  NZ  LYS B 538      10.275  31.376  21.506  1.00 55.00           N
ATOM   3865  C   LYS B 538      16.142  35.971  21.055  1.00 28.86           C
ATOM   3866  O   LYS B 538      15.915  37.005  20.425  1.00 29.11           O
ATOM   3867  N   PRO B 539      17.289  35.290  20.917  1.00 25.45           N
ATOM   3868  CD  PRO B 539      17.826  34.185  21.727  1.00 22.65           C
ATOM   3869  CA  PRO B 539      18.285  35.763  19.952  1.00 24.40           C
ATOM   3870  CB  PRO B 539      19.518  34.912  20.276  1.00 28.27           C
ATOM   3871  CG  PRO B 539      18.920  33.647  20.824  1.00 33.25           C
ATOM   3872  C   PRO B 539      17.828  35.548  18.507  1.00 28.17           C
ATOM   3873  O   PRO B 539      17.136  34.582  18.201  1.00 25.84           O
ATOM   3874  N   TYR B 540      18.229  36.458  17.630  1.00 22.91           N
ATOM   3875  CA  TYR B 540      17.918  36.423  16.206  1.00 26.70           C
ATOM   3876  CB  TYR B 540      18.740  35.333  15.518  1.00 23.59           C
ATOM   3877  CG  TYR B 540      20.240  35.373  15.839  1.00 29.92           C
ATOM   3878  CD1 TYR B 540      21.094  36.237  15.163  1.00 24.88           C
ATOM   3879  CE1 TYR B 540      22.470  36.264  15.447  1.00 24.04           C
ATOM   3880  CD2 TYR B 540      20.773  34.542  16.821  1.00 28.81           C
ATOM   3881  CE2 TYR B 540      22.153  34.568  17.142  1.00 22.99           C
ATOM   3882  CZ  TYR B 540      22.988  35.424  16.443  1.00 20.60           C
ATOM   3883  OH  TYR B 540      24.327  35.447  16.724  1.00 23.56           O
ATOM   3884  C   TYR B 540      16.435  36.134  16.017  1.00 25.23           C
ATOM   3885  O   TYR B 540      16.063  35.273  15.224  1.00 28.39           O
ATOM   3886  N   LYS B 541      15.637  36.889  16.769  1.00 28.66           N
ATOM   3887  CA  LYS B 541      14.186  36.785  16.823  1.00 40.37           C
ATOM   3888  CB  LYS B 541      13.642  38.072  17.450  1.00 43.79           C
ATOM   3889  CG  LYS B 541      12.245  37.962  18.030  1.00 55.46           C
ATOM   3890  CD  LYS B 541      11.876  39.211  18.856  1.00 55.84           C
ATOM   3891  CE  LYS B 541      12.786  39.383  20.081  1.00 60.14           C
ATOM   3892  NZ  LYS B 541      12.345  40.490  20.993  1.00 56.25           N
ATOM   3893  C   LYS B 541      13.502  36.524  15.480  1.00 43.30           C
ATOM   3894  O   LYS B 541      12.731  35.578  15.337  1.00 43.84           O
ATOM   3895  N   LYS B 542      13.791  37.349  14.493  1.00 43.89           N
ATOM   3896  CA  LYS B 542      13.147  37.178  13.200  1.00 50.62           C
ATOM   3897  CB  LYS B 542      12.893  38.547  12.575  1.00 51.21           C
ATOM   3898  CG  LYS B 542      14.153  39.355  12.339  1.00 56.73           C
ATOM   3899  CD  LYS B 542      13.849  40.636  11.571  1.00 61.48           C
ATOM   3900  CE  LYS B 542      15.135  41.350  11.161  1.00 60.94           C
ATOM   3901  NZ  LYS B 542      14.892  42.611  10.395  1.00 64.23           N
ATOM   3902  C   LYS B 542      13.921  36.309  12.221  1.00 56.90           C
ATOM   3903  O   LYS B 542      13.821  36.518  11.008  1.00 59.68           O
ATOM   3904  N   MET B 543      14.663  35.322  12.724  1.00 41.97           N
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ATOM	3905	CA	MET	B	543	15.443	34.453	11.844	1.00	45.64	C
ATOM	3906	CB	MET	B	543	16.925	34.817	11.907	1.00	43.71	C
ATOM	3907	CG	MET	B	543	17.348	35.994	11.066	1.00	53.65	C
ATOM	3908	SD	MET	B	543	19.100	36.330	11.367	1.00	42.99	S
ATOM	3909	CE	MET	B	543	18.961	37.898	12.209	1.00	45.52	C
ATOM	3910	C	MET	B	543	15.332	32.979	12.173	1.00	47.61	C
ATOM	3911	O	MET	B	543	15.075	32.599	13.318	1.00	48.77	O
ATOM	3912	N	LYS	B	544	15.562	32.152	11.157	1.00	48.07	N
ATOM	3913	CA	LYS	B	544	15.522	30.704	11.301	1.00	54.78	C
ATOM	3914	CB	LYS	B	544	14.693	30.079	10.181	1.00	55.48	C
ATOM	3915	CG	LYS	B	544	15.303	30.244	8.792	1.00	64.05	C
ATOM	3916	CD	LYS	B	544	14.493	29.491	7.739	1.00	64.50	C
ATOM	3917	CE	LYS	B	544	15.167	29.517	6.367	1.00	65.75	C
ATOM	3918	NZ	LYS	B	544	14.420	28.692	5.363	1.00	63.25	N
ATOM	3919	C	LYS	B	544	16.953	30.168	11.231	1.00	56.68	C
ATOM	3920	O	LYS	B	544	17.908	30.904	11.473	1.00	54.87	O
ATOM	3921	N	GLY	B	545	17.092	28.890	10.885	1.00	54.19	N
ATOM	3922	CA	GLY	B	545	18.408	28.280	10.805	1.00	51.15	C
ATOM	3923	C	GLY	B	545	19.352	28.912	9.797	1.00	50.65	C
ATOM	3924	O	GLY	B	545	20.219	29.694	10.174	1.00	52.75	O
ATOM	3925	N	PRO	B	546	19.213	28.585	8.504	1.00	50.84	N
ATOM	3926	CD	PRO	B	546	18.223	27.634	7.965	1.00	54.61	C
ATOM	3927	CA	PRO	B	546	20.056	29.110	7.423	1.00	51.43	C
ATOM	3928	CB	PRO	B	546	19.341	28.613	6.164	1.00	52.58	C
ATOM	3929	CG	PRO	B	546	18.809	27.294	6.609	1.00	51.61	C
ATOM	3930	C	PRO	B	546	20.241	30.624	7.416	1.00	45.67	C
ATOM	3931	O	PRO	B	546	21.274	31.128	6.963	1.00	40.66	O
ATOM	3932	N	GLU	B	547	19.234	31.343	7.903	1.00	40.50	N
ATOM	3933	CA	GLU	B	547	19.294	32.796	7.953	1.00	44.42	C
ATOM	3934	CB	GLU	B	547	17.963	33.376	8.410	1.00	44.41	C
ATOM	3935	CG	GLU	B	547	16.811	33.093	7.475	1.00	59.26	C
ATOM	3936	CD	GLU	B	547	15.538	33.763	7.927	1.00	56.22	C
ATOM	3937	OE1	GLU	B	547	15.479	35.013	7.898	1.00	62.09	O
ATOM	3938	OE2	GLU	B	547	14.603	33.037	8.319	1.00	59.62	O
ATOM	3939	C	GLU	B	547	20.391	33.282	8.902	1.00	35.91	C
ATOM	3940	O	GLU	B	547	21.149	34.172	8.555	1.00	34.83	O
ATOM	3941	N	VAL	B	548	20.460	32.694	10.094	1.00	36.33	N
ATOM	3942	CA	VAL	B	548	21.473	33.108	11.080	1.00	26.71	C
ATOM	3943	CB	VAL	B	548	21.252	32.396	12.420	1.00	35.48	C
ATOM	3944	CG1	VAL	B	548	22.285	32.872	13.448	1.00	32.82	C
ATOM	3945	CG2	VAL	B	548	19.847	32.688	12.917	1.00	40.22	C
ATOM	3946	C	VAL	B	548	22.890	32.843	10.591	1.00	31.26	C
ATOM	3947	O	VAL	B	548	23.762	33.696	10.708	1.00	33.92	O
ATOM	3948	N	MET	B	549	23.125	31.663	10.027	1.00	31.21	N
ATOM	3949	CA	MET	B	549	24.439	31.316	9.511	1.00	35.46	C
ATOM	3950	CB	MET	B	549	24.397	29.909	8.908	1.00	40.89	C
ATOM	3951	CG	MET	B	549	25.766	29.271	8.799	1.00	51.71	C
ATOM	3952	SD	MET	B	549	26.636	29.238	10.404	1.00	72.82	S
ATOM	3953	CE	MET	B	549	27.806	30.616	10.266	1.00	56.71	C
ATOM	3954	C	MET	B	549	24.918	32.325	8.445	1.00	31.51	C
ATOM	3955	O	MET	B	549	26.050	32.788	8.479	1.00	31.13	O
ATOM	3956	N	ALA	B	550	24.042	32.645	7.501	1.00	32.16	N
ATOM	3957	CA	ALA	B	550	24.373	33.588	6.431	1.00	33.32	C
ATOM	3958	CB	ALA	B	550	23.206	33.653	5.428	1.00	37.58	C
ATOM	3959	C	ALA	B	550	24.656	34.979	7.014	1.00	25.47	C
ATOM	3960	O	ALA	B	550	25.568	35.680	6.578	1.00	29.24	O
ATOM	3961	N	PHE	B	551	23.857	35.360	8.007	1.00	25.23	N
ATOM	3962	CA	PHE	B	551	23.975	36.647	8.706	1.00	28.55	C
ATOM	3963	CB	PHE	B	551	22.852	36.714	9.769	1.00	20.31	C
ATOM	3964	CG	PHE	B	551	22.783	38.000	10.543	1.00	29.64	C
ATOM	3965	CD1	PHE	B	551	22.226	39.144	9.973	1.00	28.55	C
ATOM	3966	CD2	PHE	B	551	23.209	38.052	11.876	1.00	29.88	C
ATOM	3967	CE1	PHE	B	551	22.081	40.319	10.716	1.00	26.70	C
ATOM	3968	CE2	PHE	B	551	23.066	39.232	12.636	1.00	26.29	C
ATOM	3969	CZ	PHE	B	551	22.498	40.362	12.050	1.00	31.05	C
ATOM	3970	C	PHE	B	551	25.354	36.743	9.361	1.00	26.40	C
ATOM	3971	O	PHE	B	551	26.084	37.721	9.188	1.00	22.68	O
ATOM	3972	N	ILE	B	552	25.717	35.720	10.123	1.00	23.43	N

ATOM	3973	CA	ILE	B	552	27.022	35.707	10.778	1.00 21.41	C
ATOM	3974	CB	ILE	B	552	27.135	34.460	11.681	1.00 26.93	C
ATOM	3975	CG2	ILE	B	552	28.553	34.320	12.206	1.00 28.00	C
ATOM	3976	CG1	ILE	B	552	26.046	34.533	12.764	1.00 27.40	C
ATOM	3977	CD1	ILE	B	552	26.179	35.709	13.768	1.00 29.73	C
ATOM	3978	C	ILE	B	552	28.146	35.706	9.737	1.00 22.04	C
ATOM	3979	O	ILE	B	552	29.139	36.428	9.871	1.00 25.44	O
ATOM	3980	N	GLU	B	553	27.988	34.910	8.684	1.00 25.85	N
ATOM	3981	CA	GLU	B	553	29.004	34.842	7.630	1.00 30.95	C
ATOM	3982	CB	GLU	B	553	28.613	33.796	6.580	1.00 40.19	C
ATOM	3983	CG	GLU	B	553	28.654	32.360	7.092	1.00 48.42	C
ATOM	3984	CD	GLU	B	553	30.068	31.858	7.339	1.00 49.16	C
ATOM	3985	OE1	GLU	B	553	30.212	30.786	7.970	1.00 54.92	O
ATOM	3986	OE2	GLU	B	553	31.030	32.525	6.896	1.00 56.67	O
ATOM	3987	C	GLU	B	553	29.220	36.206	6.947	1.00 29.01	C
ATOM	3988	O	GLU	B	553	30.331	36.527	6.525	1.00 34.32	O
ATOM	3989	N	GLN	B	554	28.152	36.988	6.835	1.00 30.24	N
ATOM	3990	CA	GLN	B	554	28.214	38.324	6.240	1.00 33.67	C
ATOM	3991	CB	GLN	B	554	26.806	38.870	6.010	1.00 35.02	C
ATOM	3992	CG	GLN	B	554	26.026	38.224	4.891	1.00 47.06	C
ATOM	3993	CD	GLN	B	554	24.620	38.761	4.858	1.00 45.80	C
ATOM	3994	OE1	GLN	B	554	24.410	39.970	5.004	1.00 52.95	O
ATOM	3995	NE2	GLN	B	554	23.647	37.874	4.669	1.00 52.85	N
ATOM	3996	C	GLN	B	554	28.940	39.308	7.154	1.00 35.79	C
ATOM	3997	O	GLN	B	554	29.176	40.452	6.772	1.00 29.12	O
ATOM	3998	N	GLY	B	555	29.274	38.871	8.366	1.00 26.81	N
ATOM	3999	CA	GLY	B	555	29.960	39.765	9.284	1.00 29.43	C
ATOM	4000	C	GLY	B	555	29.025	40.644	10.119	1.00 27.00	C
ATOM	4001	O	GLY	B	555	29.447	41.672	10.660	1.00 26.99	O
ATOM	4002	N	LYS	B	556	27.759	40.257	10.231	1.00 20.65	N
ATOM	4003	CA	LYS	B	556	26.826	41.024	11.045	1.00 21.47	C
ATOM	4004	CB	LYS	B	556	25.489	41.198	10.315	1.00 24.59	C
ATOM	4005	CG	LYS	B	556	25.631	41.916	8.959	1.00 24.98	C
ATOM	4006	CD	LYS	B	556	24.280	42.165	8.338	1.00 24.97	C
ATOM	4007	CE	LYS	B	556	24.429	42.911	6.990	1.00 31.95	C
ATOM	4008	NZ	LYS	B	556	23.084	43.238	6.391	1.00 32.23	N
ATOM	4009	C	LYS	B	556	26.580	40.283	12.364	1.00 22.25	C
ATOM	4010	O	LYS	B	556	26.701	39.057	12.431	1.00 21.17	O
ATOM	4011	N	ARG	B	557	26.208	41.049	13.384	1.00 20.82	N
ATOM	4012	CA	ARG	B	557	25.950	40.496	14.709	1.00 22.17	C
ATOM	4013	CB	ARG	B	557	27.164	40.778	15.629	1.00 19.79	C
ATOM	4014	CG	ARG	B	557	28.487	40.159	15.124	1.00 21.41	C
ATOM	4015	CD	ARG	B	557	28.495	38.618	15.195	1.00 19.59	C
ATOM	4016	NE	ARG	B	557	29.796	38.029	14.814	1.00 20.25	N
ATOM	4017	CZ	ARG	B	557	30.161	37.681	13.579	1.00 23.23	C
ATOM	4018	NH1	ARG	B	557	29.329	37.849	12.534	1.00 21.34	N
ATOM	4019	NH2	ARG	B	557	31.354	37.117	13.379	1.00 18.85	N
ATOM	4020	C	ARG	B	557	24.699	41.113	15.311	1.00 25.58	C
ATOM	4021	O	ARG	B	557	24.163	42.122	14.787	1.00 20.60	O
ATOM	4022	N	MET	B	558	24.211	40.520	16.405	1.00 23.12	N
ATOM	4023	CA	MET	B	558	23.031	41.057	17.061	1.00 23.08	C
ATOM	4024	CB	MET	B	558	22.577	40.150	18.226	1.00 21.21	C
ATOM	4025	CG	MET	B	558	21.929	38.861	17.759	1.00 23.06	C
ATOM	4026	SD	MET	B	558	21.172	37.972	19.155	1.00 25.40	S
ATOM	4027	CE	MET	B	558	22.589	37.274	19.959	1.00 20.17	C
ATOM	4028	C	MET	B	558	23.299	42.458	17.588	1.00 26.20	C
ATOM	4029	O	MET	B	558	24.416	42.787	18.026	1.00 22.21	O
ATOM	4030	N	GLU	B	559	22.262	43.287	17.554	1.00 22.33	N
ATOM	4031	CA	GLU	B	559	22.354	44.649	18.023	1.00 25.04	C
ATOM	4032	CB	GLU	B	559	21.047	45.392	17.711	1.00 33.85	C
ATOM	4033	CG	GLU	B	559	19.765	44.572	17.953	1.00 44.82	C
ATOM	4034	CD	GLU	B	559	19.514	43.500	16.868	1.00 56.27	C
ATOM	4035	OE1	GLU	B	559	19.120	43.868	15.733	1.00 60.02	O
ATOM	4036	OE2	GLU	B	559	19.710	42.290	17.149	1.00 44.19	O
ATOM	4037	C	GLU	B	559	22.646	44.778	19.513	1.00 25.59	C
ATOM	4038	O	GLU	B	559	22.362	43.880	20.302	1.00 29.33	O
ATOM	4039	N	CYS	B	560	23.210	45.913	19.897	1.00 22.19	N
ATOM	4040	CA	CYS	B	560	23.471	46.170	21.306	1.00 25.34	C

ATOM	4041	CB	CYS	B	560	24.313	47.440	21.454	1.00 26.43	C
ATOM	4042	SG	CYS	B	560	24.611	47.893	23.164	1.00 30.43	S
ATOM	4043	C	CYS	B	560	22.108	46.336	22.013	1.00 32.06	C
ATOM	4044	O	CYS	B	560	21.262	47.124	21.570	1.00 29.35	O
ATOM	4045	N	PRO	B	561	21.855	45.564	23.092	1.00 30.63	N
ATOM	4046	CD	PRO	B	561	22.644	44.426	23.611	1.00 28.65	C
ATOM	4047	CA	PRO	B	561	20.570	45.686	23.803	1.00 31.69	C
ATOM	4048	CB	PRO	B	561	20.727	44.723	24.987	1.00 28.11	C
ATOM	4049	CG	PRO	B	561	21.605	43.638	24.418	1.00 25.66	C
ATOM	4050	C	PRO	B	561	20.348	47.111	24.298	1.00 28.57	C
ATOM	4051	O	PRO	B	561	21.292	47.850	24.542	1.00 26.62	O
ATOM	4052	N	PRO	B	562	19.092	47.519	24.459	1.00 37.07	N
ATOM	4053	CD	PRO	B	562	17.852	46.840	24.046	1.00 39.32	C
ATOM	4054	CA	PRO	B	562	18.821	48.880	24.939	1.00 38.49	C
ATOM	4055	CB	PRO	B	562	17.294	48.942	24.948	1.00 42.66	C
ATOM	4056	CG	PRO	B	562	16.920	48.002	23.833	1.00 48.28	C
ATOM	4057	C	PRO	B	562	19.419	49.086	26.336	1.00 38.16	C
ATOM	4058	O	PRO	B	562	19.329	48.207	27.193	1.00 38.50	O
ATOM	4059	N	GLU	B	563	20.042	50.236	26.568	1.00 37.38	N
ATOM	4060	CA	GLU	B	563	20.623	50.530	27.881	1.00 43.37	C
ATOM	4061	CB	GLU	B	563	19.564	50.341	28.981	1.00 49.78	C
ATOM	4062	CG	GLU	B	563	18.309	51.190	28.805	1.00 53.84	C
ATOM	4063	CD	GLU	B	563	17.088	50.587	29.496	1.00 61.69	C
ATOM	4064	OE1	GLU	B	563	17.133	50.389	30.734	1.00 64.80	O
ATOM	4065	OE2	GLU	B	563	16.085	50.307	28.795	1.00 62.44	O
ATOM	4066	C	GLU	B	563	21.873	49.714	28.228	1.00 42.92	C
ATOM	4067	O	GLU	B	563	22.433	49.860	29.314	1.00 46.04	O
ATOM	4068	N	CYS	B	564	22.312	48.832	27.332	1.00 40.16	N
ATOM	4069	CA	CYS	B	564	23.527	48.070	27.589	1.00 35.91	C
ATOM	4070	CB	CYS	B	564	23.614	46.843	26.662	1.00 35.94	C
ATOM	4071	SG	CYS	B	564	25.157	45.907	26.802	1.00 37.39	S
ATOM	4072	C	CYS	B	564	24.706	49.006	27.324	1.00 37.21	C
ATOM	4073	O	CYS	B	564	24.832	49.559	26.231	1.00 36.78	O
ATOM	4074	N	PRO	B	565	25.580	49.200	28.324	1.00 35.01	N
ATOM	4075	CD	PRO	B	565	25.531	48.573	29.655	1.00 39.96	C
ATOM	4076	CA	PRO	B	565	26.753	50.072	28.200	1.00 32.47	C
ATOM	4077	CB	PRO	B	565	27.382	50.015	29.589	1.00 40.02	C
ATOM	4078	CG	PRO	B	565	26.960	48.666	30.098	1.00 43.81	C
ATOM	4079	C	PRO	B	565	27.709	49.607	27.127	1.00 35.02	C
ATOM	4080	O	PRO	B	565	27.860	48.403	26.893	1.00 34.15	O
ATOM	4081	N	PRO	B	566	28.396	50.558	26.475	1.00 33.68	N
ATOM	4082	CD	PRO	B	566	28.297	52.010	26.727	1.00 34.27	C
ATOM	4083	CA	PRO	B	566	29.360	50.272	25.408	1.00 30.53	C
ATOM	4084	CB	PRO	B	566	29.998	51.647	25.137	1.00 31.64	C
ATOM	4085	CG	PRO	B	566	28.908	52.607	25.481	1.00 31.51	C
ATOM	4086	C	PRO	B	566	30.412	49.223	25.792	1.00 31.72	C
ATOM	4087	O	PRO	B	566	30.757	48.379	24.978	1.00 28.48	O
ATOM	4088	N	GLU	B	567	30.920	49.285	27.028	1.00 27.33	N
ATOM	4089	CA	GLU	B	567	31.960	48.345	27.472	1.00 33.27	C
ATOM	4090	CB	GLU	B	567	32.451	48.701	28.894	1.00 36.30	C
ATOM	4091	CG	GLU	B	567	32.553	50.189	29.192	1.00 49.34	C
ATOM	4092	CD	GLU	B	567	31.195	50.835	29.391	1.00 50.90	C
ATOM	4093	OE1	GLU	B	567	30.471	50.431	30.330	1.00 63.92	O
ATOM	4094	OE2	GLU	B	567	30.851	51.744	28.612	1.00 47.96	O
ATOM	4095	C	GLU	B	567	31.440	46.908	27.485	1.00 26.60	C
ATOM	4096	O	GLU	B	567	32.143	45.964	27.089	1.00 25.31	O
ATOM	4097	N	LEU	B	568	30.208	46.747	27.948	1.00 25.52	N
ATOM	4098	CA	LEU	B	568	29.590	45.442	28.017	1.00 28.35	C
ATOM	4099	CB	LEU	B	568	28.312	45.549	28.851	1.00 31.11	C
ATOM	4100	CG	LEU	B	568	27.993	44.399	29.788	1.00 31.00	C
ATOM	4101	CD1	LEU	B	568	29.277	43.796	30.349	1.00 35.96	C
ATOM	4102	CD2	LEU	B	568	27.101	44.939	30.912	1.00 25.70	C
ATOM	4103	C	LEU	B	568	29.289	44.925	26.621	1.00 30.51	C
ATOM	4104	O	LEU	B	568	29.498	43.738	26.341	1.00 22.86	O
ATOM	4105	N	TYR	B	569	28.793	45.791	25.733	1.00 23.22	N
ATOM	4106	CA	TYR	B	569	28.538	45.310	24.383	1.00 22.95	C
ATOM	4107	CB	TYR	B	569	27.765	46.361	23.542	1.00 21.93	C
ATOM	4108	CG	TYR	B	569	27.412	45.828	22.170	1.00 21.83	C

ATOM	4109	CD1	TYR	B	569	26.583	44.721	22.022	1.00	21.17	C
ATOM	4110	CE1	TYR	B	569	26.304	44.169	20.757	1.00	22.67	C
ATOM	4111	CD2	TYR	B	569	27.966	46.396	21.006	1.00	28.53	C
ATOM	4112	CE2	TYR	B	569	27.703	45.853	19.739	1.00	27.28	C
ATOM	4113	CZ	TYR	B	569	26.881	44.746	19.622	1.00	28.33	C
ATOM	4114	OH	TYR	B	569	26.664	44.202	18.384	1.00	25.54	O
ATOM	4115	C	TYR	B	569	29.856	44.948	23.683	1.00	19.58	C
ATOM	4116	O	TYR	B	569	29.909	43.976	22.908	1.00	23.18	O
ATOM	4117	N	ALA	B	570	30.927	45.704	23.943	1.00	23.62	N
ATOM	4118	CA	ALA	B	570	32.206	45.415	23.296	1.00	24.27	C
ATOM	4119	CB	ALA	B	570	33.287	46.413	23.739	1.00	26.06	C
ATOM	4120	C	ALA	B	570	32.670	43.993	23.615	1.00	24.88	C
ATOM	4121	O	ALA	B	570	33.226	43.307	22.768	1.00	23.64	O
ATOM	4122	N	LEU	B	571	32.443	43.587	24.856	1.00	23.04	N
ATOM	4123	CA	LEU	B	571	32.844	42.259	25.336	1.00	21.51	C
ATOM	4124	CB	LEU	B	571	32.668	42.201	26.866	1.00	23.34	C
ATOM	4125	CG	LEU	B	571	32.928	40.815	27.465	1.00	22.60	C
ATOM	4126	CD1	LEU	B	571	34.295	40.301	27.028	1.00	24.30	C
ATOM	4127	CD2	LEU	B	571	32.820	40.914	28.981	1.00	24.39	C
ATOM	4128	C	LEU	B	571	31.988	41.197	24.676	1.00	16.75	C
ATOM	4129	O	LEU	B	571	32.472	40.189	24.163	1.00	20.66	O
ATOM	4130	N	MET	B	572	30.687	41.427	24.715	1.00	20.93	N
ATOM	4131	CA	MET	B	572	29.728	40.535	24.102	1.00	20.96	C
ATOM	4132	CB	MET	B	572	28.356	41.204	24.223	1.00	28.64	C
ATOM	4133	CG	MET	B	572	27.271	40.510	23.502	1.00	30.16	C
ATOM	4134	SD	MET	B	572	25.729	41.414	23.691	1.00	24.19	S
ATOM	4135	CE	MET	B	572	25.754	41.989	25.454	1.00	22.91	C
ATOM	4136	C	MET	B	572	30.117	40.358	22.625	1.00	20.33	C
ATOM	4137	O	MET	B	572	30.204	39.235	22.101	1.00	20.73	O
ATOM	4138	N	SER	B	573	30.373	41.470	21.941	1.00	18.39	N
ATOM	4139	CA	SER	B	573	30.735	41.412	20.528	1.00	21.31	C
ATOM	4140	CB	SER	B	573	30.747	42.839	19.939	1.00	25.35	C
ATOM	4141	OG	SER	B	573	31.143	42.855	18.581	1.00	27.38	O
ATOM	4142	C	SER	B	573	32.073	40.693	20.296	1.00	23.59	C
ATOM	4143	O	SER	B	573	32.231	39.962	19.324	1.00	21.82	O
ATOM	4144	N	ASP	B	574	33.043	40.889	21.176	1.00	22.93	N
ATOM	4145	CA	ASP	B	574	34.322	40.196	21.019	1.00	21.19	C
ATOM	4146	CB	ASP	B	574	35.363	40.684	22.039	1.00	21.91	C
ATOM	4147	CG	ASP	B	574	35.914	42.071	21.707	1.00	25.96	C
ATOM	4148	OD1	ASP	B	574	35.752	42.553	20.567	1.00	23.74	O
ATOM	4149	OD2	ASP	B	574	36.547	42.657	22.604	1.00	26.12	O
ATOM	4150	C	ASP	B	574	34.156	38.667	21.166	1.00	22.88	C
ATOM	4151	O	ASP	B	574	34.942	37.915	20.585	1.00	23.63	O
ATOM	4152	N	CYS	B	575	33.161	38.218	21.938	1.00	19.59	N
ATOM	4153	CA	CYS	B	575	32.906	36.778	22.097	1.00	20.12	C
ATOM	4154	CB	CYS	B	575	31.822	36.522	23.163	1.00	22.35	C
ATOM	4155	SG	CYS	B	575	32.353	36.912	24.873	1.00	23.15	S
ATOM	4156	C	CYS	B	575	32.426	36.205	20.772	1.00	22.05	C
ATOM	4157	O	CYS	B	575	32.442	34.991	20.572	1.00	19.70	O
ATOM	4158	N	TRP	B	576	32.001	37.096	19.877	1.00	20.34	N
ATOM	4159	CA	TRP	B	576	31.514	36.699	18.556	1.00	19.05	C
ATOM	4160	CB	TRP	B	576	30.184	37.393	18.208	1.00	19.93	C
ATOM	4161	CG	TRP	B	576	29.089	37.172	19.205	1.00	22.10	C
ATOM	4162	CD2	TRP	B	576	28.077	38.106	19.558	1.00	17.49	C
ATOM	4163	CE2	TRP	B	576	27.263	37.485	20.547	1.00	18.66	C
ATOM	4164	CE3	TRP	B	576	27.763	39.414	19.127	1.00	16.82	C
ATOM	4165	CD1	TRP	B	576	28.868	36.045	19.956	1.00	20.31	C
ATOM	4166	NE1	TRP	B	576	27.764	36.225	20.770	1.00	19.04	N
ATOM	4167	CZ2	TRP	B	576	26.158	38.130	21.122	1.00	19.31	C
ATOM	4168	CZ3	TRP	B	576	26.653	40.059	19.692	1.00	19.50	C
ATOM	4169	CH2	TRP	B	576	25.861	39.418	20.684	1.00	19.35	C
ATOM	4170	C	TRP	B	576	32.493	36.958	17.405	1.00	22.30	C
ATOM	4171	O	TRP	B	576	32.062	37.191	16.262	1.00	20.73	O
ATOM	4172	N	ILE	B	577	33.792	36.942	17.714	1.00	19.99	N
ATOM	4173	CA	ILE	B	577	34.826	37.103	16.689	1.00	21.32	C
ATOM	4174	CB	ILE	B	577	36.215	37.309	17.338	1.00	20.92	C
ATOM	4175	CG2	ILE	B	577	37.351	36.977	16.323	1.00	19.24	C
ATOM	4176	CG1	ILE	B	577	36.318	38.764	17.847	1.00	26.98	C

ATOM	4177	CD1	ILE	B	577	37.577	39.046	18.674	1.00	31.70	C
ATOM	4178	C	ILE	B	577	34.774	35.798	15.891	1.00	22.46	C
ATOM	4179	O	ILE	B	577	34.789	34.707	16.468	1.00	22.10	O
ATOM	4180	N	TYR	B	578	34.673	35.914	14.571	1.00	20.33	N
ATOM	4181	CA	TYR	B	578	34.532	34.751	13.715	1.00	24.28	C
ATOM	4182	CB	TYR	B	578	34.387	35.200	12.248	1.00	24.92	C
ATOM	4183	CG	TYR	B	578	33.925	34.103	11.307	1.00	25.66	C
ATOM	4184	CD1	TYR	B	578	32.574	33.963	10.977	1.00	29.87	C
ATOM	4185	CE1	TYR	B	578	32.139	32.918	10.134	1.00	32.04	C
ATOM	4186	CD2	TYR	B	578	34.831	33.173	10.770	1.00	31.85	C
ATOM	4187	CE2	TYR	B	578	34.397	32.126	9.938	1.00	29.55	C
ATOM	4188	CZ	TYR	B	578	33.047	32.009	9.628	1.00	31.34	C
ATOM	4189	OH	TYR	B	578	32.596	30.972	8.824	1.00	31.73	O
ATOM	4190	C	TYR	B	578	35.648	33.715	13.814	1.00	29.60	C
ATOM	4191	O	TYR	B	578	35.377	32.529	14.014	1.00	21.86	O
ATOM	4192	N	LYS	B	579	36.887	34.175	13.614	1.00	24.49	N
ATOM	4193	CA	LYS	B	579	38.069	33.335	13.631	1.00	27.75	C
ATOM	4194	CB	LYS	B	579	39.301	34.121	13.145	1.00	30.85	C
ATOM	4195	CG	LYS	B	579	39.212	34.623	11.695	1.00	39.76	C
ATOM	4196	CD	LYS	B	579	40.550	35.234	11.213	1.00	43.80	C
ATOM	4197	CE	LYS	B	579	40.481	35.643	9.735	1.00	52.66	C
ATOM	4198	NZ	LYS	B	579	41.684	36.457	9.328	1.00	53.08	N
ATOM	4199	C	LYS	B	579	38.346	32.811	15.021	1.00	28.50	C
ATOM	4200	O	LYS	B	579	38.585	33.568	15.942	1.00	27.27	O
ATOM	4201	N	TRP	B	580	38.335	31.495	15.128	1.00	27.56	N
ATOM	4202	CA	TRP	B	580	38.574	30.806	16.385	1.00	33.99	C
ATOM	4203	CB	TRP	B	580	38.649	29.310	16.079	1.00	33.38	C
ATOM	4204	CG	TRP	B	580	38.850	28.472	17.259	1.00	38.62	C
ATOM	4205	CD2	TRP	B	580	40.063	27.818	17.639	1.00	38.34	C
ATOM	4206	CE2	TRP	B	580	39.793	27.097	18.830	1.00	42.10	C
ATOM	4207	CE3	TRP	B	580	41.354	27.768	17.091	1.00	43.21	C
ATOM	4208	CD1	TRP	B	580	37.920	28.145	18.199	1.00	40.63	C
ATOM	4209	NE1	TRP	B	580	38.479	27.312	19.150	1.00	37.48	N
ATOM	4210	CZ2	TRP	B	580	40.767	26.333	19.484	1.00	42.20	C
ATOM	4211	CZ3	TRP	B	580	42.328	27.004	17.742	1.00	44.42	C
ATOM	4212	CH2	TRP	B	580	42.025	26.297	18.927	1.00	49.85	C
ATOM	4213	C	TRP	B	580	39.862	31.267	17.077	1.00	29.68	C
ATOM	4214	O	TRP	B	580	39.862	31.591	18.262	1.00	30.01	O
ATOM	4215	N	GLU	B	581	40.962	31.306	16.336	1.00	27.48	N
ATOM	4216	CA	GLU	B	581	42.236	31.710	16.917	1.00	27.95	C
ATOM	4217	CB	GLU	B	581	43.349	31.535	15.875	1.00	41.30	C
ATOM	4218	CG	GLU	B	581	43.080	30.409	14.878	1.00	45.98	C
ATOM	4219	CD	GLU	B	581	42.292	30.894	13.672	1.00	53.35	C
ATOM	4220	OE1	GLU	B	581	42.833	31.742	12.919	1.00	61.50	O
ATOM	4221	OE2	GLU	B	581	41.144	30.442	13.466	1.00	44.26	O
ATOM	4222	C	GLU	B	581	42.269	33.141	17.458	1.00	31.33	C
ATOM	4223	O	GLU	B	581	43.070	33.449	18.327	1.00	33.50	O
ATOM	4224	N	ASP	B	582	41.386	34.006	16.961	1.00	28.16	N
ATOM	4225	CA	ASP	B	582	41.341	35.407	17.389	1.00	24.75	C
ATOM	4226	CB	ASP	B	582	41.073	36.298	16.169	1.00	29.45	C
ATOM	4227	CG	ASP	B	582	42.179	36.201	15.131	1.00	39.01	C
ATOM	4228	OD1	ASP	B	582	43.301	35.821	15.524	1.00	35.67	O
ATOM	4229	OD2	ASP	B	582	41.937	36.495	13.937	1.00	38.00	O
ATOM	4230	C	ASP	B	582	40.307	35.726	18.478	1.00	26.77	C
ATOM	4231	O	ASP	B	582	40.250	36.848	18.993	1.00	25.92	O
ATOM	4232	N	ARG	B	583	39.487	34.744	18.816	1.00	27.16	N
ATOM	4233	CA	ARG	B	583	38.448	34.959	19.818	1.00	29.93	C
ATOM	4234	CB	ARG	B	583	37.324	33.921	19.611	1.00	23.20	C
ATOM	4235	CG	ARG	B	583	35.974	34.196	20.334	1.00	20.53	C
ATOM	4236	CD	ARG	B	583	34.993	33.051	20.050	1.00	17.55	C
ATOM	4237	NE	ARG	B	583	34.872	32.798	18.608	1.00	17.49	N
ATOM	4238	CZ	ARG	B	583	34.658	31.610	18.055	1.00	22.33	C
ATOM	4239	NH1	ARG	B	583	34.528	30.522	18.811	1.00	20.02	N
ATOM	4240	NH2	ARG	B	583	34.618	31.501	16.721	1.00	21.31	N
ATOM	4241	C	ARG	B	583	39.101	34.827	21.203	1.00	26.43	C
ATOM	4242	O	ARG	B	583	39.964	33.975	21.417	1.00	24.85	O
ATOM	4243	N	PRO	B	584	38.694	35.679	22.159	1.00	23.83	N
ATOM	4244	CD	PRO	B	584	37.731	36.791	22.028	1.00	23.73	C

ATOM	4245	CA	PRO	B	584	39.252	35.638	23.516	1.00	25.03	C
ATOM	4246	CB	PRO	B	584	38.660	36.877	24.178	1.00	25.59	C
ATOM	4247	CG	PRO	B	584	37.346	37.053	23.469	1.00	24.23	C
ATOM	4248	C	PRO	B	584	38.890	34.383	24.302	1.00	25.66	C
ATOM	4249	O	PRO	B	584	37.896	33.722	23.987	1.00	22.86	O
ATOM	4250	N	ASP	B	585	39.714	34.082	25.314	1.00	20.92	N
ATOM	4251	CA	ASP	B	585	39.492	32.946	26.205	1.00	23.08	C
ATOM	4252	CB	ASP	B	585	40.833	32.346	26.685	1.00	32.60	C
ATOM	4253	CG	ASP	B	585	41.670	31.806	25.541	1.00	38.55	C
ATOM	4254	OD1	ASP	B	585	41.153	31.012	24.727	1.00	48.57	O
ATOM	4255	OD2	ASP	B	585	42.865	32.180	25.469	1.00	55.39	O
ATOM	4256	C	ASP	B	585	38.763	33.456	27.448	1.00	20.51	C
ATOM	4257	O	ASP	B	585	38.686	34.667	27.668	1.00	23.27	O
ATOM	4258	N	PHE	B	586	38.260	32.542	28.286	1.00	21.45	N
ATOM	4259	CA	PHE	B	586	37.538	32.967	29.485	1.00	26.29	C
ATOM	4260	CB	PHE	B	586	36.795	31.794	30.151	1.00	22.81	C
ATOM	4261	CG	PHE	B	586	35.482	31.470	29.484	1.00	22.63	C
ATOM	4262	CD1	PHE	B	586	34.406	32.367	29.542	1.00	24.53	C
ATOM	4263	CD2	PHE	B	586	35.323	30.268	28.785	1.00	26.40	C
ATOM	4264	CE1	PHE	B	586	33.179	32.049	28.910	1.00	18.28	C
ATOM	4265	CE2	PHE	B	586	34.112	29.961	28.161	1.00	24.68	C
ATOM	4266	CZ	PHE	B	586	33.048	30.847	28.231	1.00	19.51	C
ATOM	4267	C	PHE	B	586	38.440	33.673	30.486	1.00	24.38	C
ATOM	4268	O	PHE	B	586	37.983	34.473	31.267	1.00	23.72	O
ATOM	4269	N	LEU	B	587	39.741	33.395	30.440	1.00	27.00	N
ATOM	4270	CA	LEU	B	587	40.650	34.114	31.337	1.00	24.91	C
ATOM	4271	CB	LEU	B	587	42.093	33.688	31.039	1.00	32.67	C
ATOM	4272	CG	LEU	B	587	43.216	34.188	31.943	1.00	40.26	C
ATOM	4273	CD1	LEU	B	587	43.348	35.672	31.784	1.00	43.71	C
ATOM	4274	CD2	LEU	B	587	42.926	33.834	33.380	1.00	40.03	C
ATOM	4275	C	LEU	B	587	40.455	35.627	31.106	1.00	23.16	C
ATOM	4276	O	LEU	B	587	40.225	36.374	32.063	1.00	26.74	O
ATOM	4277	N	THR	B	588	40.494	36.088	29.852	1.00	23.64	N
ATOM	4278	CA	THR	B	588	40.294	37.516	29.607	1.00	22.82	C
ATOM	4279	CB	THR	B	588	40.852	37.982	28.229	1.00	33.41	C
ATOM	4280	OG1	THR	B	588	40.043	37.479	27.172	1.00	46.39	O
ATOM	4281	CG2	THR	B	588	42.266	37.477	28.056	1.00	31.62	C
ATOM	4282	C	THR	B	588	38.832	37.929	29.711	1.00	22.83	C
ATOM	4283	O	THR	B	588	38.539	39.006	30.205	1.00	27.35	O
ATOM	4284	N	VAL	B	589	37.915	37.069	29.258	1.00	23.23	N
ATOM	4285	CA	VAL	B	589	36.502	37.418	29.370	1.00	23.31	C
ATOM	4286	CB	VAL	B	589	35.601	36.298	28.759	1.00	25.23	C
ATOM	4287	CG1	VAL	B	589	34.128	36.521	29.142	1.00	24.91	C
ATOM	4288	CG2	VAL	B	589	35.751	36.315	27.238	1.00	24.02	C
ATOM	4289	C	VAL	B	589	36.082	37.688	30.816	1.00	21.77	C
ATOM	4290	O	VAL	B	589	35.384	38.666	31.097	1.00	21.67	O
ATOM	4291	N	GLU	B	590	36.503	36.817	31.736	1.00	24.09	N
ATOM	4292	CA	GLU	B	590	36.158	36.986	33.149	1.00	23.44	C
ATOM	4293	CB	GLU	B	590	36.700	35.792	33.980	1.00	23.66	C
ATOM	4294	CG	GLU	B	590	36.346	35.806	35.489	1.00	28.31	C
ATOM	4295	CD	GLU	B	590	37.173	36.793	36.342	1.00	30.31	C
ATOM	4296	OE1	GLU	B	590	38.375	36.990	36.060	1.00	30.33	O
ATOM	4297	OE2	GLU	B	590	36.623	37.345	37.325	1.00	30.51	O
ATOM	4298	C	GLU	B	590	36.722	38.300	33.698	1.00	24.63	C
ATOM	4299	O	GLU	B	590	36.060	38.995	34.469	1.00	21.17	O
ATOM	4300	N	GLN	B	591	37.948	38.645	33.304	1.00	23.83	N
ATOM	4301	CA	GLN	B	591	38.550	39.896	33.775	1.00	25.38	C
ATOM	4302	CB	GLN	B	591	40.005	39.980	33.324	1.00	27.76	C
ATOM	4303	CG	GLN	B	591	40.877	38.896	33.902	1.00	36.74	C
ATOM	4304	CD	GLN	B	591	42.333	39.101	33.554	1.00	43.26	C
ATOM	4305	OE1	GLN	B	591	42.669	39.908	32.677	1.00	44.86	O
ATOM	4306	NE2	GLN	B	591	43.206	38.370	34.230	1.00	44.68	N
ATOM	4307	C	GLN	B	591	37.818	41.132	33.279	1.00	25.08	C
ATOM	4308	O	GLN	B	591	37.616	42.102	34.019	1.00	26.57	O
ATOM	4309	N	ARG	B	592	37.423	41.110	32.012	1.00	23.67	N
ATOM	4310	CA	ARG	B	592	36.712	42.239	31.437	1.00	25.80	C
ATOM	4311	CB	ARG	B	592	36.631	42.087	29.917	1.00	23.30	C
ATOM	4312	CG	ARG	B	592	38.018	42.247	29.276	1.00	31.02	C

ATOM	4313	CD	ARG	B	592	38.006	41.980	27.792	1.00	31.50	C
ATOM	4314	NE	ARG	B	592	37.163	42.935	27.079	1.00	25.46	N
ATOM	4315	CZ	ARG	B	592	36.913	42.861	25.781	1.00	24.58	C
ATOM	4316	NH1	ARG	B	592	37.446	41.880	25.069	1.00	25.78	N
ATOM	4317	NH2	ARG	B	592	36.127	43.760	25.206	1.00	26.82	N
ATOM	4318	C	ARG	B	592	35.326	42.323	32.039	1.00	25.35	C
ATOM	4319	O	ARG	B	592	34.803	43.415	32.284	1.00	25.98	O
ATOM	4320	N	MET	B	593	34.722	41.165	32.293	1.00	23.15	N
ATOM	4321	CA	MET	B	593	33.380	41.176	32.867	1.00	24.63	C
ATOM	4322	CB	MET	B	593	32.774	39.764	32.822	1.00	22.51	C
ATOM	4323	CG	MET	B	593	31.324	39.697	33.218	1.00	22.94	C
ATOM	4324	SD	MET	B	593	30.230	40.679	32.086	1.00	29.24	S
ATOM	4325	CE	MET	B	593	29.463	41.710	33.269	1.00	27.63	C
ATOM	4326	C	MET	B	593	33.442	41.705	34.297	1.00	25.96	C
ATOM	4327	O	MET	B	593	32.582	42.480	34.719	1.00	28.48	O
ATOM	4328	N	ARG	B	594	34.459	41.296	35.044	1.00	23.96	N
ATOM	4329	CA	ARG	B	594	34.605	41.743	36.417	1.00	24.96	C
ATOM	4330	CB	ARG	B	594	35.849	41.106	37.042	1.00	23.17	C
ATOM	4331	CG	ARG	B	594	36.061	41.480	38.522	1.00	25.85	C
ATOM	4332	CD	ARG	B	594	37.401	40.946	39.044	1.00	37.38	C
ATOM	4333	NE	ARG	B	594	37.415	39.490	39.157	1.00	42.96	N
ATOM	4334	CZ	ARG	B	594	36.932	38.814	40.201	1.00	43.14	C
ATOM	4335	NH1	ARG	B	594	36.400	39.464	41.232	1.00	47.77	N
ATOM	4336	NH2	ARG	B	594	36.966	37.488	40.206	1.00	41.23	N
ATOM	4337	C	ARG	B	594	34.707	43.271	36.461	1.00	27.20	C
ATOM	4338	O	ARG	B	594	34.071	43.930	37.291	1.00	29.00	O
ATOM	4339	N	ALA	B	595	35.499	43.827	35.548	1.00	29.98	N
ATOM	4340	CA	ALA	B	595	35.709	45.271	35.455	1.00	32.90	C
ATOM	4341	CB	ALA	B	595	36.814	45.570	34.424	1.00	33.21	C
ATOM	4342	C	ALA	B	595	34.423	46.010	35.087	1.00	33.52	C
ATOM	4343	O	ALA	B	595	34.139	47.075	35.627	1.00	31.72	O
ATOM	4344	N	CYS	B	596	33.646	45.439	34.166	1.00	31.09	N
ATOM	4345	CA	CYS	B	596	32.389	46.044	33.750	1.00	32.73	C
ATOM	4346	CB	CYS	B	596	31.768	45.264	32.585	1.00	31.31	C
ATOM	4347	SG	CYS	B	596	32.614	45.490	30.999	1.00	41.27	S
ATOM	4348	C	CYS	B	596	31.412	46.053	34.907	1.00	33.26	C
ATOM	4349	O	CYS	B	596	30.741	47.055	35.158	1.00	31.15	O
ATOM	4350	N	TYR	B	597	31.326	44.925	35.604	1.00	28.78	N
ATOM	4351	CA	TYR	B	597	30.415	44.811	36.736	1.00	29.03	C
ATOM	4352	CB	TYR	B	597	30.465	43.384	37.311	1.00	30.58	C
ATOM	4353	CG	TYR	B	597	29.811	43.233	38.665	1.00	31.39	C
ATOM	4354	CD1	TYR	B	597	28.548	43.773	38.917	1.00	33.23	C
ATOM	4355	CE1	TYR	B	597	27.957	43.673	40.186	1.00	36.25	C
ATOM	4356	CD2	TYR	B	597	30.465	42.579	39.702	1.00	36.29	C
ATOM	4357	CE2	TYR	B	597	29.884	42.466	40.977	1.00	42.36	C
ATOM	4358	CZ	TYR	B	597	28.634	43.021	41.210	1.00	40.23	C
ATOM	4359	OH	TYR	B	597	28.091	42.957	42.474	1.00	40.28	O
ATOM	4360	C	TYR	B	597	30.758	45.825	37.827	1.00	32.53	C
ATOM	4361	O	TYR	B	597	29.871	46.537	38.335	1.00	33.59	O
ATOM	4362	N	TYR	B	598	32.036	45.883	38.179	1.00	30.77	N
ATOM	4363	CA	TYR	B	598	32.508	46.793	39.218	1.00	38.97	C
ATOM	4364	CB	TYR	B	598	34.012	46.604	39.460	1.00	39.06	C
ATOM	4365	CG	TYR	B	598	34.385	45.365	40.244	1.00	40.81	C
ATOM	4366	CD1	TYR	B	598	35.714	45.111	40.590	1.00	48.71	C
ATOM	4367	CE1	TYR	B	598	36.075	43.943	41.281	1.00	48.51	C
ATOM	4368	CD2	TYR	B	598	33.424	44.423	40.612	1.00	47.38	C
ATOM	4369	CE2	TYR	B	598	33.771	43.259	41.298	1.00	46.97	C
ATOM	4370	CZ	TYR	B	598	35.098	43.024	41.626	1.00	49.34	C
ATOM	4371	OH	TYR	B	598	35.445	41.854	42.264	1.00	48.67	O
ATOM	4372	C	TYR	B	598	32.227	48.230	38.823	1.00	43.37	C
ATOM	4373	O	TYR	B	598	31.873	49.057	39.667	1.00	48.95	O
ATOM	4374	N	SER	B	599	32.379	48.535	37.541	1.00	37.43	N
ATOM	4375	CA	SER	B	599	32.122	49.872	37.055	1.00	43.16	C
ATOM	4376	CB	SER	B	599	32.529	49.961	35.590	1.00	43.45	C
ATOM	4377	OG	SER	B	599	32.332	51.262	35.090	1.00	53.97	O
ATOM	4378	C	SER	B	599	30.636	50.205	37.223	1.00	45.93	C
ATOM	4379	O	SER	B	599	30.271	51.316	37.617	1.00	40.00	O
ATOM	4380	N	LEU	B	600	29.773	49.240	36.935	1.00	39.11	N

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ATOM   4381  CA  LEU B 600      28.337  49.462  37.065  1.00 44.57           C
ATOM   4382  CB  LEU B 600      27.552  48.395  36.295  1.00 38.25           C
ATOM   4383  CG  LEU B 600      27.711  48.441  34.770  1.00 42.03           C
ATOM   4384  CD1 LEU B 600      27.111  47.196  34.147  1.00 37.50           C
ATOM   4385  CD2 LEU B 600      27.039  49.683  34.214  1.00 45.85           C
ATOM   4386  C   LEU B 600      27.897  49.456  38.516  1.00 43.73           C
ATOM   4387  O   LEU B 600      26.980  50.191  38.892  1.00 46.87           O
ATOM   4388  N   ALA B 601      28.556  48.628  39.323  1.00 40.69           N
ATOM   4389  CA  ALA B 601      28.242  48.478  40.741  1.00 47.37           C
ATOM   4390  CB  ALA B 601      29.065  47.346  41.335  1.00 46.75           C
ATOM   4391  C   ALA B 601      28.506  49.775  41.498  1.00 52.65           C
ATOM   4392  O   ALA B 601      27.834  50.082  42.483  1.00 53.31           O
ATOM   4393  N   SER B 602      29.492  50.527  41.021  1.00 52.09           N
ATOM   4394  CA  SER B 602      29.860  51.804  41.617  1.00 57.33           C
ATOM   4395  CB  SER B 602      31.346  52.069  41.381  1.00 58.94           C
ATOM   4396  OG  SER B 602      32.141  51.082  42.020  1.00 59.82           O
ATOM   4397  C   SER B 602      29.024  52.912  40.981  1.00 59.94           C
ATOM   4398  O   SER B 602      29.388  54.086  41.029  1.00 64.66           O
ATOM   4399  N   LYS B 603      27.900  52.515  40.389  1.00 62.33           N
ATOM   4400  CA  LYS B 603      26.974  53.425  39.720  1.00 64.02           C
ATOM   4401  CB  LYS B 603      26.569  54.555  40.673  1.00 64.16           C
ATOM   4402  CG  LYS B 603      25.091  54.908  40.626  1.00 65.22           C
ATOM   4403  CD  LYS B 603      24.767  55.995  41.635  1.00 64.28           C
ATOM   4404  CE  LYS B 603      23.270  56.270  41.693  1.00 67.89           C
ATOM   4405  NZ  LYS B 603      22.949  57.422  42.589  1.00 67.06           N
ATOM   4406  C   LYS B 603      27.609  53.996  38.446  1.00 65.47           C
ATOM   4407  O   LYS B 603      27.032  53.798  37.352  1.00 66.51           O
ATOM   4408  OXT LYS B 603      28.685  54.625  38.551  1.00 68.34           O
TER       1      LYS B 603
ATOM   4409  O4  STU C 995      10.701  -7.072  -3.088  1.00 26.93           O
ATOM   4410  C25 STU C 995      11.180  -5.863  -3.690  1.00 23.34           C
ATOM   4411  C24 STU C 995      10.859  -4.664  -2.680  1.00 29.45           C
ATOM   4412  C23 STU C 995      10.138  -5.127  -1.364  1.00 22.89           C
ATOM   4413  C22 STU C 995       8.878  -5.986  -1.697  1.00 25.16           C
ATOM   4414  C21 STU C 995       9.461  -7.275  -2.433  1.00 26.44           C
ATOM   4415  C26 STU C 995       9.777  -8.334  -1.360  1.00 25.18           C
ATOM   4416  N2  STU C 995       8.422  -7.719  -3.422  1.00 23.09           N
ATOM   4417  C18 STU C 995       8.412  -7.138  -4.747  1.00 21.71           C
ATOM   4418  C19 STU C 995       9.290  -6.274  -5.405  1.00 24.08           C
ATOM   4419  C6  STU C 995       9.064  -5.832  -6.736  1.00 22.57           C
ATOM   4420  C7  STU C 995       7.866  -6.422  -7.405  1.00 25.97           C
ATOM   4421  C10 STU C 995       7.050  -7.293  -6.788  1.00 23.03           C
ATOM   4422  C11 STU C 995       7.275  -7.726  -5.438  1.00 20.70           C
ATOM   4423  C12 STU C 995       6.603  -8.591  -4.523  1.00 24.72           C
ATOM   4424  C17 STU C 995       7.298  -8.588  -3.264  1.00 25.22           C
ATOM   4425  C16 STU C 995       6.820  -9.373  -2.193  1.00 26.63           C
ATOM   4426  C15 STU C 995       5.671 -10.131  -2.339  1.00 28.90           C
ATOM   4427  C14 STU C 995       4.957 -10.136  -3.585  1.00 27.59           C
ATOM   4428  C13 STU C 995       5.443  -9.364  -4.643  1.00 24.26           C
ATOM   4429  C9  STU C 995       5.906  -7.701  -7.728  1.00 24.86           C
ATOM   4430  N1  STU C 995       6.283  -6.914  -8.894  1.00 26.80           N
ATOM   4431  C8  STU C 995       7.390  -6.161  -8.794  1.00 24.42           C
ATOM   4432  O5  STU C 995       7.870  -5.431  -9.638  1.00 25.22           O
ATOM   4433  C5  STU C 995      10.084  -4.899  -7.090  1.00 21.94           C
ATOM   4434  C20 STU C 995      10.927  -4.761  -5.943  1.00 28.12           C
ATOM   4435  C1  STU C 995      12.071  -3.894  -5.922  1.00 27.73           C
ATOM   4436  C2  STU C 995      12.350  -3.175  -7.097  1.00 30.27           C
ATOM   4437  C3  STU C 995      11.500  -3.313  -8.263  1.00 28.96           C
ATOM   4438  C4  STU C 995      10.403  -4.161  -8.243  1.00 26.89           C
ATOM   4439  N3  STU C 995      10.433  -5.565  -4.940  1.00 23.33           N
ATOM   4440  O6  STU C 995       8.116  -5.181  -2.652  1.00 24.62           O
ATOM   4441  C27 STU C 995       6.704  -5.144  -2.385  1.00 24.32           C
ATOM   4442  N4  STU C 995       9.777  -3.833  -0.560  1.00 24.88           N
ATOM   4443  C28 STU C 995       9.296  -4.199   0.820  1.00 26.60           C
TER       1      STU C 995
ATOM   4444  O4  STU D 996      14.841  21.718  34.032  1.00 26.13           O
ATOM   4445  C25 STU D 996      14.373  22.920  34.632  1.00 22.93           C
ATOM   4446  C24 STU D 996      14.706  24.128  33.610  1.00 28.10           C
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ATOM   4447  C23 STU D 996      15.417  23.644  32.288  1.00 24.94           C
ATOM   4448  C22 STU D 996      16.665  22.776  32.631  1.00 23.21           C
ATOM   4449  C21 STU D 996      16.072  21.495  33.377  1.00 27.43           C
ATOM   4450  C26 STU D 996      15.756  20.434  32.323  1.00 26.04           C
ATOM   4451  N2  STU D 996      17.133  21.077  34.359  1.00 21.43           N
ATOM   4452  C18 STU D 996      17.120  21.637  35.688  1.00 20.69           C
ATOM   4453  C19 STU D 996      16.275  22.524  36.330  1.00 23.53           C
ATOM   4454  C6  STU D 996      16.487  22.957  37.663  1.00 22.38           C
ATOM   4455  C7  STU D 996      17.682  22.366  38.337  1.00 26.78           C
ATOM   4456  C10 STU D 996      18.504  21.518  37.720  1.00 22.89           C
ATOM   4457  C11 STU D 996      18.270  21.070  36.370  1.00 19.86           C
ATOM   4458  C12 STU D 996      18.952  20.227  35.457  1.00 22.51           C
ATOM   4459  C17 STU D 996      18.237  20.202  34.206  1.00 25.41           C
ATOM   4460  C16 STU D 996      18.719  19.424  33.133  1.00 26.19           C
ATOM   4461  C15 STU D 996      19.869  18.670  33.275  1.00 28.16           C
ATOM   4462  C14 STU D 996      20.600  18.678  34.521  1.00 25.48           C
ATOM   4463  C13 STU D 996      20.112  19.449  35.580  1.00 23.07           C
ATOM   4464  C9  STU D 996      19.647  21.104  38.659  1.00 23.46           C
ATOM   4465  N1  STU D 996      19.276  21.887  39.826  1.00 25.16           N
ATOM   4466  C8  STU D 996      18.166  22.640  39.728  1.00 22.97           C
ATOM   4467  O5  STU D 996      17.688  23.365  40.576  1.00 23.93           O
ATOM   4468  C5  STU D 996      15.472  23.870  38.015  1.00 23.02           C
ATOM   4469  C20 STU D 996      14.631  24.010  36.865  1.00 26.41           C
ATOM   4470  C1  STU D 996      13.476  24.883  36.850  1.00 25.65           C
ATOM   4471  C2  STU D 996      13.208  25.595  38.019  1.00 30.69           C
ATOM   4472  C3  STU D 996      14.057  25.459  39.181  1.00 27.27           C
ATOM   4473  C4  STU D 996      15.157  24.612  39.158  1.00 26.75           C
ATOM   4474  N3  STU D 996      15.112  23.212  35.878  1.00 22.92           N
ATOM   4475  O6  STU D 996      17.429  23.573  33.576  1.00 23.16           O
ATOM   4476  C27 STU D 996      18.832  23.642  33.286  1.00 24.37           C
ATOM   4477  N4  STU D 996      15.802  24.935  31.463  1.00 23.94           N
ATOM   4478  C28 STU D 996      16.275  24.547  30.090  1.00 24.01           C
TER       1      STU D 996
ATOM   4479  OH2 TIP S   1       0.421   4.204  13.673  1.00 22.10           O
ATOM   4480  OH2 TIP S   2       0.033   9.184  13.707  1.00 21.18           O
ATOM   4481  OH2 TIP S   3      11.945  -2.213   0.210  1.00 22.87           O
ATOM   4482  OH2 TIP S   4      25.132  33.017  17.239  1.00 22.45           O
ATOM   4483  OH2 TIP S   5      25.496  37.992  17.154  1.00 20.79           O
ATOM   4484  OH2 TIP S   6     -12.049 -13.944  12.451  1.00 22.33           O
ATOM   4485  OH2 TIP S   7      14.395   8.858  57.889  1.00 29.61           O
ATOM   4486  OH2 TIP S   8      13.627  26.578  30.735  1.00 22.89           O
ATOM   4487  OH2 TIP S   9      11.059 -19.955 -26.913  1.00 28.80           O
ATOM   4488  OH2 TIP S  10      29.070  27.910  20.630  1.00 25.77           O
ATOM   4489  OH2 TIP S  11      -3.520  -0.809  10.277  1.00 25.06           O
ATOM   4490  OH2 TIP S  12      18.345  30.239  26.486  1.00 23.39           O
ATOM   4491  OH2 TIP S  13       1.869  14.815  18.471  1.00 23.60           O
ATOM   4492  OH2 TIP S  14      35.075  25.727  28.589  1.00 28.87           O
ATOM   4493  OH2 TIP S  15       7.227   1.385   4.419  1.00 22.68           O
ATOM   4494  OH2 TIP S  16      -9.560  -3.026   2.397  1.00 27.48           O
ATOM   4495  OH2 TIP S  17      -5.464  -3.857   7.924  1.00 23.68           O
ATOM   4496  OH2 TIP S  18      -6.496   8.745  20.202  1.00 23.82           O
ATOM   4497  OH2 TIP S  19      -2.873  -2.292   5.603  1.00 23.16           O
ATOM   4498  OH2 TIP S  20     -11.803   8.285  18.254  1.00 24.29           O
ATOM   4499  OH2 TIP S  21      28.416  26.453  25.290  1.00 23.25           O
ATOM   4500  OH2 TIP S  22      37.391  37.035  12.669  1.00 26.06           O
ATOM   4501  OH2 TIP S  23     -17.573  -7.098   4.343  1.00 27.79           O
ATOM   4502  OH2 TIP S  24      32.073  37.514  10.731  1.00 24.94           O
ATOM   4503  OH2 TIP S  25      13.480  31.449  36.563  1.00 25.71           O
ATOM   4504  OH2 TIP S  26     -14.437   9.362  17.730  1.00 32.36           O
ATOM   4505  OH2 TIP S  27      35.416  25.457  18.662  1.00 25.28           O
ATOM   4506  OH2 TIP S  28      31.029  24.811  22.942  1.00 25.60           O
ATOM   4507  OH2 TIP S  29      -9.872  -3.294  12.263  1.00 25.74           O
ATOM   4508  OH2 TIP S  30      26.467   9.752  17.607  1.00 27.17           O
ATOM   4509  OH2 TIP S  31       6.790  -6.857   1.076  1.00 30.39           O
ATOM   4510  OH2 TIP S  32      40.010  38.095  13.209  1.00 33.16           O
ATOM   4511  OH2 TIP S  33      34.735  13.425  28.194  1.00 29.80           O
ATOM   4512  OH2 TIP S  34      -9.205 -15.364   2.764  1.00 26.99           O
ATOM   4513  OH2 TIP S  35      -0.980 -18.986  13.270  1.00 26.43           O
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ATOM	4514	OH2	TIP	S	36	24.213	18.114	34.694	1.00	29.43	O
ATOM	4515	OH2	TIP	S	37	1.416	-10.764	-3.798	1.00	29.81	O
ATOM	4516	OH2	TIP	S	38	43.144	21.699	26.548	1.00	30.26	O
ATOM	4517	OH2	TIP	S	39	-14.848	7.171	-3.854	1.00	30.65	O
ATOM	4518	OH2	TIP	S	40	39.180	42.936	36.141	1.00	31.31	O
ATOM	4519	OH2	TIP	S	41	40.406	35.919	34.784	1.00	30.00	O
ATOM	4520	OH2	TIP	S	42	0.420	2.218	15.485	1.00	29.77	O
ATOM	4521	OH2	TIP	S	43	35.271	29.926	13.265	1.00	31.24	O
ATOM	4522	OH2	TIP	S	44	12.095	2.647	-5.592	1.00	26.76	O
ATOM	4523	OH2	TIP	S	45	-9.718	1.172	17.653	1.00	30.07	O
ATOM	4524	OH2	TIP	S	46	-3.404	14.594	13.732	1.00	30.39	O
ATOM	4525	OH2	TIP	S	47	18.726	21.922	29.867	1.00	32.07	O
ATOM	4526	OH2	TIP	S	48	13.555	7.866	51.920	1.00	39.23	O
ATOM	4527	OH2	TIP	S	49	28.975	43.404	17.200	1.00	29.02	O
ATOM	4528	OH2	TIP	S	50	-13.569	14.156	-5.246	1.00	33.70	O
ATOM	4529	OH2	TIP	S	51	26.355	20.255	28.832	1.00	29.58	O
ATOM	4530	OH2	TIP	S	52	9.161	10.323	16.585	1.00	35.40	O
ATOM	4531	OH2	TIP	S	53	-0.757	-8.626	2.106	1.00	29.81	O
ATOM	4532	OH2	TIP	S	54	-14.070	-4.107	6.620	1.00	27.24	O
ATOM	4533	OH2	TIP	S	55	11.946	-20.893	-21.008	1.00	43.13	O
ATOM	4534	OH2	TIP	S	56	25.189	30.969	15.454	1.00	29.79	O
ATOM	4535	OH2	TIP	S	57	36.813	31.260	38.289	1.00	31.14	O
ATOM	4536	OH2	TIP	S	58	-11.290	2.441	-7.391	1.00	30.15	O
ATOM	4537	OH2	TIP	S	59	9.218	10.129	12.339	1.00	32.37	O
ATOM	4538	OH2	TIP	S	60	16.469	39.110	14.335	1.00	36.98	O
ATOM	4539	OH2	TIP	S	61	39.600	24.658	24.347	1.00	28.57	O
ATOM	4540	OH2	TIP	S	62	40.886	19.814	39.523	1.00	31.30	O
ATOM	4541	OH2	TIP	S	63	28.663	25.506	21.907	1.00	28.05	O
ATOM	4542	OH2	TIP	S	64	16.334	39.034	18.587	1.00	30.97	O
ATOM	4543	OH2	TIP	S	65	-4.453	-10.056	-10.600	1.00	35.01	O
ATOM	4544	OH2	TIP	S	66	30.644	48.610	22.338	1.00	34.83	O
ATOM	4545	OH2	TIP	S	67	29.080	17.008	23.184	1.00	42.53	O
ATOM	4546	OH2	TIP	S	68	20.437	-8.985	-8.586	1.00	30.66	O
ATOM	4547	OH2	TIP	S	69	-3.136	-3.317	8.937	1.00	26.92	O
ATOM	4548	OH2	TIP	S	70	-3.528	-11.754	7.661	1.00	42.36	O
ATOM	4549	OH2	TIP	S	71	-14.052	9.990	-6.784	1.00	36.91	O
ATOM	4550	OH2	TIP	S	72	13.280	20.389	48.150	1.00	37.12	O
ATOM	4551	OH2	TIP	S	73	39.598	27.291	23.321	1.00	29.86	O
ATOM	4552	OH2	TIP	S	74	-14.000	-1.419	7.609	1.00	29.52	O
ATOM	4553	OH2	TIP	S	75	12.287	-8.370	-17.212	1.00	38.16	O
ATOM	4554	OH2	TIP	S	76	0.127	-2.062	7.336	1.00	31.92	O
ATOM	4555	OH2	TIP	S	77	39.657	38.747	37.688	1.00	35.97	O
ATOM	4556	OH2	TIP	S	78	6.921	10.871	13.240	1.00	39.95	O
ATOM	4557	OH2	TIP	S	79	3.173	20.739	-5.925	1.00	36.12	O
ATOM	4558	OH2	TIP	S	80	2.499	-2.849	7.192	1.00	37.12	O
ATOM	4559	OH2	TIP	S	81	-5.087	20.010	8.545	1.00	36.89	O
ATOM	4560	OH2	TIP	S	82	25.391	26.672	23.460	1.00	34.04	O
ATOM	4561	OH2	TIP	S	83	23.029	25.932	23.668	1.00	37.18	O
ATOM	4562	OH2	TIP	S	84	13.382	-6.941	-0.286	1.00	40.85	O
ATOM	4563	OH2	TIP	S	85	27.715	12.569	29.074	1.00	44.29	O
ATOM	4564	OH2	TIP	S	86	29.990	18.665	41.491	1.00	37.50	O
ATOM	4565	OH2	TIP	S	87	22.380	49.448	36.934	1.00	39.98	O
ATOM	4566	OH2	TIP	S	88	18.662	39.652	17.714	1.00	39.70	O
ATOM	4567	OH2	TIP	S	89	40.100	17.469	30.708	1.00	36.01	O
ATOM	4568	OH2	TIP	S	90	-14.239	11.528	5.631	1.00	40.89	O
ATOM	4569	OH2	TIP	S	91	15.281	18.913	57.001	1.00	45.15	O
ATOM	4570	OH2	TIP	S	92	15.691	-4.194	-6.244	1.00	46.89	O
ATOM	4571	OH2	TIP	S	93	-5.712	-9.326	5.564	1.00	28.37	O
ATOM	4572	OH2	TIP	S	94	12.167	21.855	31.241	1.00	41.68	O
ATOM	4573	OH2	TIP	S	95	-3.343	-17.247	16.589	1.00	36.78	O
ATOM	4574	OH2	TIP	S	96	11.156	23.711	33.209	1.00	35.57	O
ATOM	4575	OH2	TIP	S	97	25.545	16.245	18.621	1.00	42.42	O
ATOM	4576	OH2	TIP	S	98	40.918	18.920	34.722	1.00	45.15	O
ATOM	4577	OH2	TIP	S	99	11.862	37.569	22.369	1.00	39.52	O
ATOM	4578	OH2	TIP	S	100	15.658	8.162	-3.968	1.00	36.43	O
ATOM	4579	OH2	TIP	S	101	9.902	24.553	37.142	1.00	45.39	O
ATOM	4580	OH2	TIP	S	102	6.314	-5.317	-19.652	1.00	42.39	O
ATOM	4581	OH2	TIP	S	103	41.337	39.304	18.249	1.00	43.68	O

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ATOM   4582  OH2 TIP S 104       1.800  -8.520  -5.551  1.00 35.38           O
ATOM   4583  OH2 TIP S 105      -2.162 -16.185   1.874  1.00 43.33           O
ATOM   4584  OH2 TIP S 106      39.849  40.296  25.274  1.00 39.96           O
ATOM   4585  OH2 TIP S 107      17.812  14.377  26.537  1.00 49.82           O
ATOM   4586  OH2 TIP S 108      20.087  16.149  58.833  1.00 41.90           O
ATOM   4587  OH2 TIP S 109      23.681  20.283  36.450  1.00 34.15           O
ATOM   4588  OH2 TIP S 110      31.232  19.396  25.383  1.00 31.15           O
ATOM   4589  OH2 TIP S 111       9.926  36.917  34.935  1.00 39.68           O
ATOM   4590  OH2 TIP S 112      13.742   8.657   8.468  1.00 37.13           O
ATOM   4591  OH2 TIP S 113      14.444  -5.155  -2.332  1.00 34.36           O
ATOM   4592  OH2 TIP S 114     -14.505 -11.350   0.205  1.00 38.40           O
ATOM   4593  OH2 TIP S 115     -14.458   0.142   5.499  1.00 35.12           O
ATOM   4594  OH2 TIP S 116      -0.021 -12.439  12.153  1.00 43.53           O
ATOM   4595  OH2 TIP S 117      28.916  11.485  14.387  1.00 40.27           O
ATOM   4596  OH2 TIP S 118      -4.527  10.289  -9.542  1.00 45.18           O
ATOM   4597  OH2 TIP S 119       1.974  14.755 -11.306  1.00 47.77           O
ATOM   4598  OH2 TIP S 120     -15.749  10.668  12.672  1.00 45.53           O
ATOM   4599  OH2 TIP S 121     -11.214  -2.226 -11.345  1.00 46.10           O
ATOM   4600  OH2 TIP S 122      36.682  45.523  28.569  1.00 37.78           O
ATOM   4601  OH2 TIP S 123      19.320  23.480  50.684  1.00 40.47           O
ATOM   4602  OH2 TIP S 124     -15.435  -9.919  -3.811  1.00 41.21           O
ATOM   4603  OH2 TIP S 125      38.588  26.717  13.793  1.00 44.52           O
ATOM   4604  OH2 TIP S 126       7.685 -14.424   4.306  1.00 51.58           O
ATOM   4605  OH2 TIP S 127      36.734  26.561  42.263  1.00 44.35           O
ATOM   4606  OH2 TIP S 128      23.012  18.699  64.427  1.00 55.43           O
ATOM   4607  OH2 TIP S 129     -11.079  16.753   2.337  1.00 36.15           O
ATOM   4608  OH2 TIP S 130      32.804  36.247   8.025  1.00 46.53           O
ATOM   4609  OH2 TIP S 131       5.452 -12.666 -27.857  1.00 46.24           O
ATOM   4610  OH2 TIP S 132       5.777  -5.213   4.878  1.00 52.94           O
ATOM   4611  OH2 TIP S 133      17.902  43.584  22.888  1.00 38.79           O
ATOM   4612  OH2 TIP S 134      41.529  41.359  30.489  1.00 45.08           O
ATOM   4613  OH2 TIP S 135      19.433  49.428  35.071  1.00 36.73           O
ATOM   4614  OH2 TIP S 136      40.681  17.939  17.861  1.00 52.60           O
ATOM   4615  OH2 TIP S 137       7.694  14.779   8.016  1.00 38.37           O
ATOM   4616  OH2 TIP S 138      43.631  21.569  35.087  1.00 42.92           O
ATOM   4617  OH2 TIP S 139     -14.096  -4.522   2.725  1.00 38.87           O
ATOM   4618  OH2 TIP S 140      39.647  24.357  28.138  1.00 37.44           O
ATOM   4619  OH2 TIP S 141      34.792  45.810  26.786  1.00 33.97           O
ATOM   4620  OH2 TIP S 142      35.678  30.939  40.741  1.00 50.18           O
ATOM   4621  OH2 TIP S 143       1.690  -5.943   7.932  1.00 46.04           O
ATOM   4622  OH2 TIP S 144      16.446   8.323  29.203  1.00 43.29           O
ATOM   4623  OH2 TIP S 145       4.806  -6.139 -16.268  1.00 46.89           O
ATOM   4624  OH2 TIP S 146       9.706   7.514 -13.847  1.00 40.39           O
ATOM   4625  OH2 TIP S 147      -2.757  -8.476  20.990  1.00 44.56           O
ATOM   4626  OH2 TIP S 148      19.924  51.030  32.912  1.00 56.09           O
ATOM   4627  OH2 TIP S 149      -9.256  17.012   4.187  1.00 37.40           O
ATOM   4628  OH2 TIP S 150      13.798  12.721   1.801  1.00 41.15           O
ATOM   4629  OH2 TIP S 151     -16.062  12.522   0.503  1.00 45.91           O
ATOM   4630  OH2 TIP S 152      43.042  24.814  30.118  1.00 45.63           O
ATOM   4631  OH2 TIP S 153      32.777  49.012  32.108  1.00 49.84           O
ATOM   4632  OH2 TIP S 154      35.924  45.614  31.001  1.00 42.83           O
ATOM   4633  OH2 TIP S 155      -4.339 -23.117  -0.551  1.00 49.33           O
ATOM   4634  OH2 TIP S 156      19.827  23.697  25.905  1.00 53.14           O
ATOM   4635  OH2 TIP S 157      37.820  44.919  22.145  1.00 44.38           O
ATOM   4636  OH2 TIP S 158      40.593  29.995  32.300  1.00 31.52           O
ATOM   4637  OH2 TIP S 159     -15.055   1.168  -1.359  1.00 30.62           O
ATOM   4638  OH2 TIP S 160     -16.412   7.003   5.433  1.00 32.94           O
ATOM   4639  OH2 TIP S 161      15.985  29.616  25.353  1.00 32.77           O
ATOM   4640  OH2 TIP S 162      42.076  35.832  25.453  1.00 35.51           O
ATOM   4641  OH2 TIP S 163      10.339  -9.751 -25.987  1.00 46.65           O
ATOM   4642  OH2 TIP S 164      34.356  38.780  10.727  1.00 36.90           O
ATOM   4643  OH2 TIP S 165       9.618   0.824   5.500  1.00 35.38           O
ATOM   4644  OH2 TIP S 166      26.940   9.884  20.217  1.00 38.88           O
ATOM   4645  OH2 TIP S 167      -7.023   7.631  22.982  1.00 45.13           O
ATOM   4646  OH2 TIP S 168     -17.523  -3.768   0.764  1.00 47.38           O
ATOM   4647  OH2 TIP S 169      34.610  28.019  11.023  1.00 41.98           O
ATOM   4648  OH2 TIP S 170      38.500  22.241  10.888  1.00 49.86           O
ATOM   4649  OH2 TIP S 171      39.773  16.186  22.302  1.00 42.81           O
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ATOM   4650  OH2 TIP S 172      39.007  29.639  38.711  1.00 40.01           O
ATOM   4651  OH2 TIP S 173      -3.162 -13.972   1.056  1.00 37.80           O
ATOM   4652  OH2 TIP S 174      15.866  36.292  44.854  1.00 41.03           O
ATOM   4653  OH2 TIP S 175      28.716  14.934  29.871  1.00 40.86           O
ATOM   4654  OH2 TIP S 176      12.877   7.462  40.598  1.00 50.68           O
ATOM   4655  OH2 TIP S 177       6.133  20.704  -4.054  1.00 39.16           O
ATOM   4656  OH2 TIP S 178      39.969  28.942  25.391  1.00 38.15           O
ATOM   4657  OH2 TIP S 179     -13.449   0.920  -7.668  1.00 44.30           O
ATOM   4658  OH2 TIP S 180      -1.907 -19.850 -13.019  1.00 46.61           O
ATOM   4659  OH2 TIP S 181     -11.803   7.776  20.873  1.00 44.08           O
ATOM   4660  OH2 TIP S 182      15.943  16.779  25.867  1.00 50.71           O
ATOM   4661  OH2 TIP S 183      11.887  41.459  29.150  1.00 40.31           O
ATOM   4662  OH2 TIP S 184     -12.916  -6.604  20.001  1.00 48.89           O
ATOM   4663  OH2 TIP S 185      37.386  36.717  10.040  1.00 47.31           O
ATOM   4664  OH2 TIP S 186       2.834  18.279  41.221  1.00 54.64           O
ATOM   4665  OH2 TIP S 187      -9.066  -0.690  19.812  1.00 43.53           O
ATOM   4666  OH2 TIP S 188      16.454  33.980  25.756  1.00 38.52           O
ATOM   4667  OH2 TIP S 189      23.851  22.769  22.843  1.00 48.45           O
ATOM   4668  OH2 TIP S 190     -14.255 -12.614   8.773  1.00 46.74           O
ATOM   4669  OH2 TIP S 191      -5.249 -12.948 -12.695  1.00 53.90           O
ATOM   4670  OH2 TIP S 192       9.039 -20.611   1.774  1.00 42.77           O
ATOM   4671  OH2 TIP S 193      -5.304  -5.892 -10.918  1.00 47.95           O
ATOM   4672  OH2 TIP S 194       9.516 -11.723   5.016  1.00 49.40           O
ATOM   4673  OH2 TIP S 195      20.372  36.265   6.690  1.00 42.55           O
ATOM   4674  OH2 TIP S 196       9.099   5.271   5.043  1.00 40.29           O
ATOM   4675  OH2 TIP S 197      28.290  20.438   9.887  1.00 44.18           O
ATOM   4676  OH2 TIP S 198      41.403  24.242  26.360  1.00 41.99           O
ATOM   4677  OH2 TIP S 199      17.555  -7.280  -3.972  1.00 45.72           O
ATOM   4678  OH2 TIP S 200      11.643  26.387  33.558  1.00 44.67           O
ATOM   4679  OH2 TIP S 201     -13.080  -2.043  17.068  1.00 48.89           O
ATOM   4680  OH2 TIP S 202      21.406  41.180   6.510  1.00 47.83           O
ATOM   4681  OH2 TIP S 203      -3.647 -14.349   4.372  1.00 45.03           O
ATOM   4682  OH2 TIP S 204       1.975 -16.444   0.528  1.00 46.05           O
ATOM   4683  OH2 TIP S 205      29.352  38.318  42.802  1.00 39.18           O
ATOM   4684  OH2 TIP S 206      23.761  43.491  42.218  1.00 52.21           O
ATOM   4685  OH2 TIP S 207      37.832  29.664  12.655  1.00 40.31           O
ATOM   4686  OH2 TIP S 208       4.964  17.602   2.226  1.00 49.67           O
ATOM   4687  OH2 TIP S 209      39.168  40.024  22.519  1.00 48.01           O
ATOM   4688  OH2 TIP S 210      13.868 -18.464  -3.462  1.00 45.96           O
ATOM   4689  OH2 TIP S 211     -15.848  -4.527   4.594  1.00 44.75           O
ATOM   4690  OH2 TIP S 212     -10.372  16.898  -0.055  1.00 41.74           O
ATOM   4691  OH2 TIP S 213      -3.769   9.428 -11.859  1.00 41.64           O
ATOM   4692  OH2 TIP S 214     -12.248  16.128   8.702  1.00 42.97           O
ATOM   4693  OH2 TIP S 215     -10.705  -1.226 -13.945  1.00 46.83           O
ATOM   4694  OH2 TIP S 216      22.402   4.106  44.758  1.00 42.90           O
ATOM   4695  OH2 TIP S 217     -17.355   1.265   1.310  1.00 49.40           O
ATOM   4696  OH2 TIP S 218      42.477  37.616  23.340  1.00 42.07           O
ATOM   4697  OH2 TIP S 219     -16.918   8.816   7.795  1.00 46.92           O
ATOM   4698  OH2 TIP S 220      27.500   8.859  43.884  1.00 48.46           O
ATOM   4699  OH2 TIP S 221      30.021  39.029  40.447  1.00 44.55           O
ATOM   4700  OH2 TIP S 222      39.391  18.850  37.190  1.00 52.09           O
ATOM   4701  OH2 TIP S 223       4.533 -18.856   1.922  1.00 50.69           O
ATOM   4702  OH2 TIP S 224      29.183  14.389  26.673  1.00 47.97           O
ATOM   4703  OH2 TIP S 225     -18.903  -8.822  10.919  1.00 49.49           O
ATOM   4704  OH2 TIP S 226      29.080  14.271  21.460  1.00 41.94           O
ATOM   4705  OH2 TIP S 227     -12.418  15.936  -7.420  1.00 49.12           O
ATOM   4706  OH2 TIP S 228      40.908  38.798  10.820  1.00 48.24           O
ATOM   4707  OH2 TIP S 229      20.873  22.585  47.103  1.00 50.53           O
ATOM   4708  OH2 TIP S 230      21.831 -10.033  -6.237  1.00 53.05           O
ATOM   4709  OH2 TIP S 231      29.823   5.586  31.413  1.00 52.07           O
ATOM   4710  OH2 TIP S 232      44.472  19.890  19.952  1.00 49.75           O
ATOM   4711  OH2 TIP S 233     -14.590 -13.479  12.084  1.00 44.70           O
ATOM   4712  OH2 TIP S 234      36.315  29.168   8.598  1.00 49.27           O
ATOM   4713  OH2 TIP S 235      -3.492 -14.586   9.423  1.00 44.24           O
ATOM   4714  OH2 TIP S 236      37.931  44.730  38.212  1.00 52.70           O
ATOM   4715  OH2 TIP S 237     -13.540  11.244   8.565  1.00 48.15           O
ATOM   4716  OH2 TIP S 238     -15.408  10.000  20.145  1.00 50.07           O
ATOM   4717  OH2 TIP S 239      20.743   2.608  48.382  1.00 49.86           O
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ATOM   4718  OH2 TIP S 240      23.597  12.310  30.357  1.00 48.72           O
ATOM   4719  OH2 TIP S 241      -5.755  -8.661 -12.899  1.00 51.10           O
ATOM   4720  OH2 TIP S 242      40.644  44.705  34.483  1.00 51.24           O
ATOM   4721  OH2 TIP S 243      32.880  11.239  31.811  1.00 48.34           O
ATOM   4722  OH2 TIP S 244      -7.454 -17.415  -0.915  1.00 45.03           O
ATOM   4723  OH2 TIP S 245      13.922  -2.398  -2.504  1.00 46.83           O
ATOM   4724  OH2 TIP S 246       0.782  12.427 -14.770  1.00 48.57           O
ATOM   4725  OH2 TIP S 247     -15.049  15.812  -3.622  1.00 51.01           O
ATOM   4726  OH2 TIP S 248       4.404  15.313  18.746  1.00 47.05           O
ATOM   4727  OH2 TIP S 249      31.402  20.217  43.758  1.00 52.57           O
ATOM   4728  OH2 TIP S 250     -10.062   2.073  -9.809  1.00 50.33           O
ATOM   4729  OH2 TIP S 251      11.650  -0.830   4.614  1.00 50.82           O
ATOM   4730  OH2 TIP S 252      -1.232 -15.435   4.563  1.00 50.12           O
ATOM   4731  OH2 TIP S 253     -12.330   0.786  18.255  1.00 43.46           O
ATOM   4732  OH2 TIP S 254      36.403  27.682  44.769  1.00 51.60           O
ATOM   4733  OH2 TIP S 255     -18.273   6.055   3.212  1.00 51.88           O
ATOM   4734  OH2 TIP S 256     -13.609  16.893  -0.632  1.00 50.05           O
ATOM   4735  OH2 TIP S 257      14.001  15.235   0.255  1.00 48.29           O
ATOM   4736  OH2 TIP S 258      10.461   2.911   6.999  1.00 51.70           O
ATOM   4737  OH2 TIP S 259      11.740  10.308  34.387  1.00 49.96           O
ATOM   4738  OH2 TIP S 260     -11.901   5.018  -8.016  1.00 50.95           O
ATOM   4739  OH2 TIP S 261     -10.492  19.957  -5.817  1.00 45.58           O
TER       1      TIP S 261
END
```

Table 2. Crystal Data and X-Ray Data Statistics

Number of crystals	1
Space group	P1 (primitive triclinic)
Unit cell dimensions	a = 35.77 b = 57.56 c = 80.20Å
	α = 68.97 β = 89.83 γ = 89.95°
Number of monomers / a.u.	2
Packing coefficient	2.05Å^3/Da
Solvent content	38%
Resolution range	50 – 1.9Å
Number of observations	386926
Number of reject observations	24465
Number of unique reflections	46855
Mosaicity	0.817
Overall	
Data redundancy	8.25
Data completeness	97.0%
$< I/\sigma (I)>$	20.6
R_{merge}	0.049
Highest resolution shell	
Resolution range	1.97-1.90Å
Completeness for shell	96.5%
R_{merge} for shell	0.175
Reflections with $I \geq 3\sigma(I)$	86.7%

Table 3. Refinement Statistics

Data used in refinement	
- resolution range	19.26-1.90Å
- intensity cutoff (Sigma(F))	0.0
- number of reflections	45463
- completeness (working +test set)	96.7%
-test set	5.0%
Fit to data used in refinement	
- overall R_{cryst}	0.182
- overall R_{free}	0.209
Fit in the highest resolution bin	
- resolution range	2.02 - 1.90 Å
- bin completeness (working +test set)	93.7%
- bin R_{cryst}	0.195
- bin R_{free}	0.241
Number of non-hydrogen atoms	
- protein atoms	4478
- ligand (2 molecules staurosporin)	70
- waters	261
Overall B value from Wilson plot	24.1Å^2
Overall mean B value	35.0Å^2
Cross-validated estimated coordinate error (low res. cutoff: 5.0Å)	
- from Luzzati plot	0.22Å
- from σ_A	0.11Å
Rms deviations from ideal values	
- bond lengths	0.011Å
- bond angles	1.3°
- dihedral angles	21.4°
- improper angles	0.91°

Table 4. List of Contacts Between Catalytic Domain of ZAP-70 and Staurosporine

atom in protein	atom in staurosporine	distance (A)	
LEU 344 O	STU C25	3.4	
GLY 345 CA	STU O4	3.5	
CYS 346 O	STU C26	3.9	
GLY 347 N	STU C26	5.4	
PHE 349 CZ	STU C16	4.5	
VAL 352 CG2	STU C17	3.8	
ALA 367 CB	STU N1	3.2	
LYS 369 CD	STU C14	4.3	
GLU 386 OE2	STU C14	4.4	
VAL 399 CG1	STU C9	4.1	
MET 414 CE	STU C13	3.6	
GLU 415 O	STU N1	3.0	H-bridge
MET 416 CA	STU O5	3.4	
ALA 417 N	STU O5	2.7	H-bridge
GLY 418 O	STU C3	4.3	
GLY 419 C	STU C3	4.8	
GLY 420 CA	STU C3	3.5	
PRO 421 CG	STU C24	3.8	
HIS 423 NE2	STU N4	5.1	through Solv3
Lys 424 NZ	STU N4	6.4	through Solv3
ARG 465 O	STU N4	3.0	H-bridge
ASN 466 OD1	STU C27	3.4	
LEU 468 CD1	STU C7	3.3	
SER 478 OG	STU C27	3.1	Alt. Pos.
ASP 479 CG	STU C15	3.5	

SEQUENCE LISTING

<110> Geiser, Martin
Ostermeier, Christian
Ramage, Paul
Zenke, Gerhard

<120> Three-Dimensional Structure of the Catalytic Domain of ZAP-70 Protein Tyrosine Kinase, Methods and Use Thereof

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        35                  40                  45

Ser Leu Val His Asp Val Arg Phe His His Phe Pro Ile Glu Arg Gln
    50                  55                  60

Leu Asn Gly Thr Tyr Ala Ile Ala Gly Gly Lys Ala His Cys Gly Pro
65                  70                  75                  80

Ala Glu Leu Cys Glu Phe Tyr Ser Arg Asp Pro Asp Gly Leu Pro Cys
                85                  90                  95

Asn Leu Arg Lys Pro Cys Asn Arg Pro Ser Gly Leu Glu Pro Gln Pro
            100                 105                 110

Gly Val Phe Asp Cys Leu Arg Asp Ala Met Val Arg Asp Tyr Val Arg
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Leu Tyr Ser Gly Ala Gln Thr Asp Gly Lys Phe Leu Leu Arg Pro Arg
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Tyr His Tyr Leu Ile Ser Gln Asp Lys Ala Gly Lys Tyr Cys Ile Pro
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His Pro Ser Thr Leu Thr His Pro Gln Arg Arg Ile Asp Thr Leu Asn
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Ser Asp Gly Tyr Thr Pro Glu Pro Ala Arg Ile Thr Ser Pro Asp Lys
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Pro Arg Pro Met Pro Met Asp Thr Ser Val Tyr Glu Ser Pro Tyr Ser
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Asp Pro Glu Glu Leu Lys Asp Lys Lys Leu Phe Leu Lys Arg Asp Asn
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Ile Pro Val Ser Asn Val Ala Glu Leu Leu His Gln Val Ser Met Gly
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        35                  40                  45

Cys Gly Asn Phe Gly Ser Val Arg Gln Gly Val Tyr Arg Met Arg Lys
    50                  55                  60

Lys Gln Ile Asp Val Ala Ile Lys Val Leu Lys Gln Gly Thr Glu Lys
65                  70                  75                  80

Ala Asp Thr Glu Glu Met Met Arg Glu Ala Gln Ile Met His Gln Leu
                85                  90                  95

Asp Asn Pro Tyr Ile Val Arg Leu Ile Gly Val Cys Gln Ala Glu Ala
            100                 105                 110

Leu Met Leu Val Met Glu Met Ala Gly Gly Gly Pro Leu His Lys Phe
        115                 120                 125

Leu Val Gly Lys Arg Glu Glu Ile Pro Val Ser Asn Val Ala Glu Leu
    130                 135                 140

Leu His Gln Val Ser Met Gly Met Lys Tyr Leu Glu Glu Lys Asn Phe
145                 150                 155                 160

Val His Arg Asp Leu Ala Ala Arg Asn Val Leu Leu Val Asn Arg His
                165                 170                 175

Tyr Ala Lys Ile Ser Asp Phe Gly Leu Ser Lys Ala Leu Gly Ala Asp
            180                 185                 190

Asp Ser Tyr Tyr Thr Ala Arg Ser Ala Gly Lys Trp Pro Leu Lys Trp
        195                 200                 205

Tyr Ala Pro Glu Cys Ile Asn Phe Arg Lys Phe Ser Ser Arg Ser Asp
    210                 215                 220

Val Trp Ser Tyr Gly Val Thr Met Trp Glu Ala Leu Ser Tyr Gly Gln
225                 230                 235                 240

Lys Pro Tyr Lys Lys Met Lys Gly Pro Glu Val Met Ala Phe Ile Glu
                245                 250                 255

Gln Gly Lys Arg Met Glu Cys Pro Pro Glu Cys Pro Pro Glu Leu Tyr
            260                 265                 270

Ala Leu Met Ser Asp Cys Trp Ile Tyr Lys Trp Glu Asp Arg Pro Asp
        275                 280                 285

Phe Leu Thr Val Glu Gln Arg Met Arg Ala Cys Tyr Tyr Ser Leu Ala
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